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This publication contains a number of Department of Defense research mission success stories enabled by high performance computing. The work was supported by many DoD laboratories and sponsors and represents 9 computational technology areas from 16 science and technology laboratories. Most of the enabling HPC was provided by DoD's HPC Modernization Program using 7 of its shared resource centers and 7 other HPC centers. The success stories were chosen to illustrate the crucial role of HPC in basic and applied research at both DoD laboratories and supporting academic and contractor participants.

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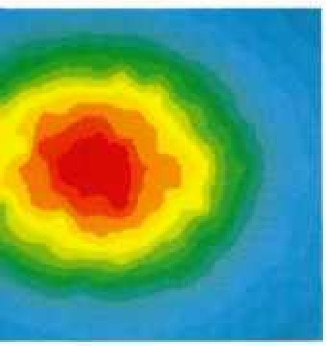
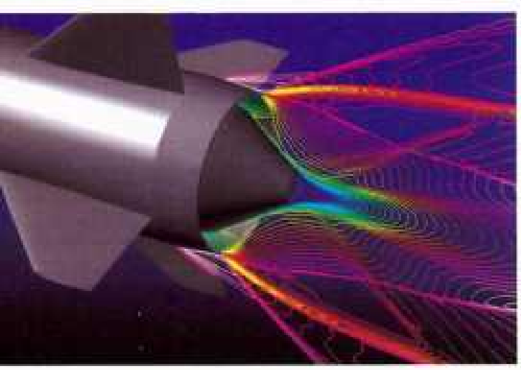
contributions to

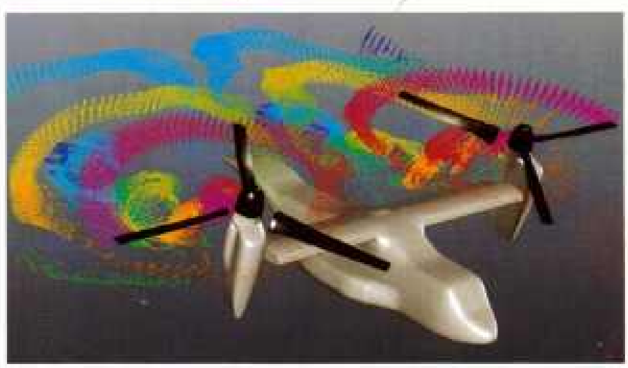
DoD Mission Success

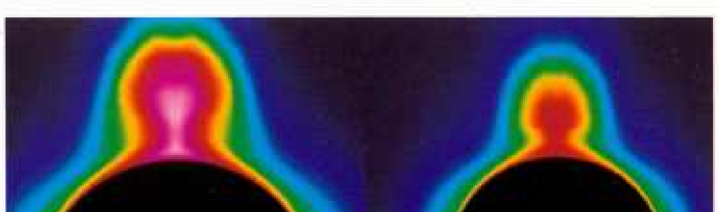
from High Performance Computing - March 1995

A report by the DoD High Performance Computing Modernization Office
Office of Secretary of Defense
Director of Defense Research and Engineering









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Anthony Pressley
Program Manager
DoD HPC Modernization Office

ADDITIONAL COPIES AND DOCUMENTATION

Additional copies of this publication may be ordered from the Defense Technical Information Center, (703) 274-6871.

Continuation of the DoD High Performance Computing Modernization Plan is discussed in a separate report, "Department of Defense High Performance Computing Modernization Plan," June 1994, available from the Defense Technical Information Center, AD 285359.

contributions to

DoD Mission Success

from High Performance Computing — March 1995

HPC ENABLES DoD SCIENCE AND TECHNOLOGY MISSION SUCCESS

Introduction

HPC ENABLES DoD SCIENCE AND TECHNOLOGY MISSION SUCCESS — Introduction

High performance computing (HPC) plays a crucial enabling role for DoD scientists and engineers. The DoD HPC Modernization Program (HPCMP) critically impacts the conduct of science and technology as well as test and evaluation initiatives by integrating, deploying, and maintaining technologically superior advanced computing and communications capabilities. The HPCMP acquires these advanced capabilities as a major contribution to defense system research, design, and development. These HPC capabilities also significantly cut defense system costs by shortening the design cycle and reducing reliance on expensive and destructive live fire and model testing. In its first year of operation, the HPCMP has provided computational resources that have already yielded improved results for scientists and engineers solving DoD mission problems.

The HPCMP creates a high performance computing environment that provides DoD scientists and engineers the resources needed to successfully execute their mission. They can access complete HPC facilities from their workstations to either their local sites or remote locations across the nation through the highest commercially available networks.

This report contains an extensive selection of abstracts of DoD mission research successes enabled by both the new DoD HPCMP systems and a few other systems. The abstracts are chosen to illustrate the role of HPC in both basic and applied research, by both DoD laboratories and supporting academic and contractor participants, and to both warfighting and civilian sector purposes.

COMPUTATIONAL TECHNOLOGY IN DoD

The research abstracted in this report ranges from fundamental or basic research, such as quantum mechanical analysis of the structures and properties of molecules and atoms, to very applied research, such as evaluating ship design decisions. The spectrum between these two extremes is dense. The difference in objectives across this spectrum must be appreciated to understand the research mission successes reported. Toward this end, the research reports follow a standard format:

Computer Resource — identifies the specific high performance computer that enabled the research and the DoD or other site that provided the HPC

Research Objective — identifies the research objective in terms of basic or applied goals

Methodology — what and why (hardware, algorithm, scalability, scalable efficiency, critical element

Results — to research objective and to computational science, if any

Significance — to basic science, the DoD mission, and the civilian sector

The success stories are organized into the following nine computational technology areas (CTAs):

Computational Structural Mechanics (CSM)

- High-resolution multi-dimensional modeling of materials and structures subjected to a broad range of impulsive loading that ranges from weak to intense.

- DoD application areas include conventional underwater explosion and ship response, structural acoustics, coupled field problems, space debris, propulsion systems, structural analysis, total weapon simulation, lethality/survivability of weapon systems (e.g., aircraft, ships, submarines, tanks), theater missile defense lethality analysis, optimization techniques, and real-time, large-scale soldier- and hardware-in-the-loop, ground vehicle dynamic simulation.

Computational Fluid Dynamics (CFD)

- Accurate numerical solution of the equations describing fluid and gas motion and the related use of digital computers in fluid dynamics research.

- For basic studies of fluid dynamics, for engineering design of complex flow configurations, for predicting the interactions of chemistry with fluid flow for combustion and propulsion, for interpreting and analyzing experimental data, and for extrapolating into regimes that are inaccessible or too costly to study.

- Encompasses all velocity regimes and scales of interest to the DoD without restrictions on the geometry and motion of boundaries defining the flow.

- The physics to be considered may entail additional force fields, coupling to surface physics and microphysics, changes of phase, changes of chemical composition, and interactions among multiple phases in heterogeneous flows.

Computational Chemistry and Materials Science (CCM)

- Quantum chemistry and molecular dynamics methods are used to design new chemical systems for fuels, lubricants, explosives, rocket propellants, catalysts, and chemical defense agents.

- Solid state modeling techniques are employed in the development of new high-performance materials for electronics, optical computing, advanced sensors, aircraft engines and structures, semiconductor lasers, laser protection systems, advanced rocket engine components, and biomedical applications.

- These computational research tools are also used to predict basic properties of new chemical species and materials that may be difficult or impossible to obtain experimentally, such as molecular geometries and energies, spectroscopic constants, intermolecular forces, reaction potential energy surfaces, and mechanical properties.

Computational Electromagnetics and Acoustics (CEA)

- High-resolution multi-dimensional solutions of Maxwell's equations to define the electromagnetic fields about antenna arrays; electromagnetic signatures of tactical ground, air, sea, and space vehicles; electromagnetic performance and design factors for EM gun technology; electromagnetic signature of buried munitions; high-power microwave performance; and the interdisciplinary applications in magnetohydrodynamics and laser systems.

- High-resolution multi-dimensional solutions of the acoustic wave equations in solids, fluids, and gases to model the acoustic fields for surveillance and communication, seismic fields for mine detection, and the acoustic shock waves of explosions for anti-personnel weapons.

Climate/Weather/Ocean Modeling (CWO)

- Modeling of the Earth's climate and weather to improve scientific understanding of the oceanic and atmospheric dynamics and developing an oceanic and atmospheric prediction capability for both military operations (safety of flight, mission, planning, optimal aircraft, ship routing, weapon system design) and civilian applications (fisheries forecast, pollutant tracking, global change studies, and weather forecasts).

- Modeling of various properties of the ocean (temperature, salinity, currents) to improve the processing gain for acoustic anti-submarine warfare (ASW)

Signal/Image Processing (SIP)

- Extraction of useful information from sensor outputs (sonar, radar, imaging, signal intelligence (SIGINT), navigation) in real time.

- Usually such processors are aboard deployable military systems and hence require ruggedized packaging and minimum size, weight, and power.

- Research, evaluation, and test of the latest signal processing concepts directed toward these embedded applications.

Forces Modeling and Simulation/C^{4}I (FMS)

- Use of command, control, communications, computers, and intelligence (C^{4}I) resources to manage a battle space.

- Faster-than-real-time, large-scale simulations of complex military engagements to facilitate mission rehearsal, mission planning, and post-mission analysis.

- Collaborative planning/replanning to support real-time operation decision-making.

- Implementation and use of digital library technology on parallel machines to support FMS/C^{4}I research and development activities.

Environmental Quality Modeling and Simulation (EQM)

- High-resolution three-dimensional Navier-Stokes modeling of hydrodynamics and contaminant and multi-constituent fate/transport through the aquatic and terrestrial ecosystem and wetland subsystems, their coupled hydrogeologic pathways, and their interconnections with numerous biological species.
- Used for stewardship and conservation of natural and cultural resources, optimal design and operation of installation restoration, and enhancement alternatives and development of short- and long-term strategies for integrated management in support of installation environmental quality.
- Work in the area of noise evaluation and abatement as well as water quality models.

Computational Electronics and Nanoelectronics (CEN)

- Variety of CAD/CAE and predictive modeling and simulation techniques.
- Areas of investigation include but are not limited to circuit and device simulation/optimization, interconnect and packaging analysis, neural networks and formal design methods, statistical analysis and design, design for test, and fault modeling.

HPCMP SHARED RESOURCE CENTERS

The DoD HPC Shared Resource Centers (SRCs) are key to the DoD HPC Modernization Program. Research described in this report has primarily been conducted using SRCs deployed in FY93. Additional deployments are underway in FY94 and FY95; see statement about additional documentation in box on inside front cover. The FY93 installed systems and sites include the following:

- Cray C90/16/512 and Y-MP8/8/128 at Army Corps of Engineers Waterways Experiment Station (CEWES), Vicksburg, MS (upgraded to 1024 MW in FY94)
- Intel Paragon XP/S-15 at Aeronautical Systems Center (ASC), Wright-Patterson AFB, OH
- Intel Paragon XP/S-25 at Naval Command, Control and Ocean Surveillance Center (NRaD), San Diego, CA
- IBM SP1 and SP2 at Maui High Performance Computing Center (MHPCC) (supporting AF Maui Optical Station (AMOS)), Kihei, HI
- Kendall Square Research KSR1-256 at Army Research Laboratory (ARL), Aberdeen Proving Ground, MD
- Thinking Machines Corporation CM-5E and CM-200 at Naval Research Laboratory (NRL), Washington, DC
- Thinking Machines Corporation CM-5 at Army High Performance Computing Research Center (AHPCRC), Minneapolis, MN.

Other high-performance computers used in support of research results reported here include the following:

- Cray 2 at Army Tank Automotive Command (TACOM), Warren, MI
- Cray 2 at Army Research Laboratory (ARL), Aberdeen Proving Ground, MD
- Cray M-98 at Arctic Region Supercomputing Center (ARSC), University of Alaska, Fairbanks, AK.
- Cray Y-MP/8/8/128 at Naval Oceanographic Office (NAVO), Stennis Space Center, MS
- Cray Y-MP and Cray M-98 (DNA) at Los Alamos National Laboratory, NM
- Cray C-90 at NASA-Ames, Moffett Field, CA
- Intel iPSC/860 at Naval Research Laboratory (NRL), Washington, DC

LABORATORIES/CENTERS RESPONSIBLE FOR REPORTED RESEARCH

Army

Army Research Office (ARO), Research Triangle Park, NC
Army Research Laboratory (ARL), Aberdeen Proving Ground, MD
Army Corps of Engineers, Waterways Experiment Station (CEWES), Vicksburg, MS
Tank Automotive Command (TACOM), Warren, MI
Armament Research, Development, and Engineering Command (ARDEC), Picatinny Arsenal, NJ
Natick Research, Development, and Engineering Center (NRDEC), Natick, MA
Army Aeroflightdynamics Directorate, Aviation and Troop Command (ATCOM), Moffett Field, CA

Navy

Office of Naval Research (ONR), Arlington, VA
Naval Surface Warfare Center (NSWC), Bethesda, MD; Silver Spring, MD; Portsmouth, VA
Naval Command, Control and Ocean Surveillance Center (NRaD), San Diego, CA
Naval Research Laboratory (NRL), Washington, DC; Stennis Space Center, MS; Monterey, CA
Naval Undersea Warfare Center (NUWC), New London, CT; Newport, RI
Naval Sea Systems Command (NAVSEA), Washington, DC

Air Force

Air Force Office of Scientific Research (AFOSR), Washington, DC
Wright Laboratory (WL), Wright-Patterson AFB, OH
Phillips Laboratory (PL), Edwards AFB, CA; Hanscom AFB, MA; Kirtland AFB, NM
Rome Laboratory (RL), Rome, NY

Defense Nuclear Agency (DNA)

CONTRIBUTIONS TO DoD MISSION SUCCESS FROM HPC

List

CONTRIBUTIONS TO DoD MISSION SUCCESS FROM HPC — List

Computational Structural Mechanics (CSM)

Computational Fluid Dynamics (CFD)

39 Torpedo Launch Dynamics — R. Ramamurti, W.C. Sandberg, R. Löhner, and J. Schwemin [Navy, NRL/DC, ONR, NUWC]

40 Projectile with Wrap-around Fins — H.L. Edge and N. Patel [Army, ARL]

41 Tools for Improved Aerodynamic Design — J.A. Burns, E.M. Cliff, and M.D. Gunzburger [Air Force, Virginia Polytechnic Institute and State University, AFOSR]

42 Supersonic Compressible Turbulence — L.D. Kral and J.F. Donovan [Air Force, McDonnell Douglas Corporation, AFOSR]

43 Compressible Turbulence — D.D. Knight [Air Force, Rutgers University, AFOSR]

44 Largest Simulation of Homogeneous Compressible Turbulence — D.H. Porter, P. Woodward, and S. Anderson [Army, ARO]

45 Large Ram Air Parachutes — S.K. Aliabadi, W. Garrard, V. Kalro, S. Mittal, T.E. Tezduyar, and K. Stein [Army, AHPCRC, ARO, NRDEC]

46 Finite-Element Methodologies for Advanced Injector Design — G.P. Wren, S.E. Ray, and T.E. Tezduyar [Army, ARL, AHPCRC, ARO]

47 Fuel-Air Mixing Enhanced by Shock-induced Vortices — D. Gottlieb, W.-S. Don, C.-W. Shu, and C. Quillen [Air Force, Brown University, AFOSR]

48 Scattering and Dissipation of Waves by Turbulence — D.G. Dommermuth and R.C.Y. Mui [Navy, Science Applications International Corporation, ONR]

49 Initial Stages of a Microbreaking Wave — D.G. Dommermuth and R.C.Y. Mui [Navy, Science Applications International Corporation, ONR]

50 Development of a Coupled CFD/CSD Methodology — J.D. Baum, Hong Luo, and R. Löhner [DNA]

51 Turbulent Mixing in Explosions — A.L. Kuhl, J.B. Bell, R.E. Ferguson, and J.P. Collins [Navy, NSWC; DNA]

52 Reactive Flow Simulations with Detailed Chemistry — J.W. Weber, Jr., E.S. Oran, and J.D. Anderson, Jr. [Air Force, Wright Laboratory, University of Maryland, AFOSR; Navy, NRL/DC]

53 Reflected-Shock/Boundary-Layer Interaction in Shock Tubes — Y.S. Weber, E.S. Oran, J.P. Boris, and J.D. Anderson, Jr. [Air Force, Wright Laboratory, University of Maryland, AFOSR; Navy, NRL/DC]

54 Three-dimensional Radiation Transport Hydrodynamics — D.E. Fyfe, J.P. Dahlburg, and J.H. Gardner [Navy, NRL/DC]

55 Time-Varying Flames — C.R. Kaplan [Navy, NRL/DC]

56 Two-dimensional Version of Sabot Discard — B.K. Edgar, S. Anderson, P. Woodward, and Kurt Fickie [Army, AHPCRC, ARO, ARL]

57 Design of Compact Exhaust Nozzles for Turbine Missile Engines — M.K. Lockwood and W.Z. Strang [Air Force, Wright Laboratory]

Computational Chemistry and Materials Science (CCM)

Computational Electromagnetics and Acoustics (CEA)

Climate/Weather/Ocean Modeling (CWO)

CONTRIBUTIONS TO DoD MISSION SUCCESS FROM HPC

Research Reports

Computational Structural Mechanics

Recent advances in high-performance computing and numerical methods have led to more accurate simulations of physical phenomena. Historically, increments in the performance and utility of HPC systems have fostered the incorporation of more complex physics and numerics into models that yield high-fidelity simulations. The DoD's HPC applications in Computational Structural Mechanics are diverse. They illustrate the paramount role HPC plays in both the development of advanced technologies as well as the evaluation of various design alternatives as an integral component of DoD's R&D programs.

The CSM contributions that follow span a broad spectrum of DoD mission requirements that include, among others, improved structural integrity for shock-hardened class of coastal mine hunters and advanced structural modeling for designing next generation weapon systems, ships, and submarines.

Mr. Kent Kimsey
Army Research Laboratory
CTA Leader for CSM

Multimode Warhead Mechanics

Ernest L. Baker
U.S. Army Armament RD&E Center, Picatinny Arsenal, NJ

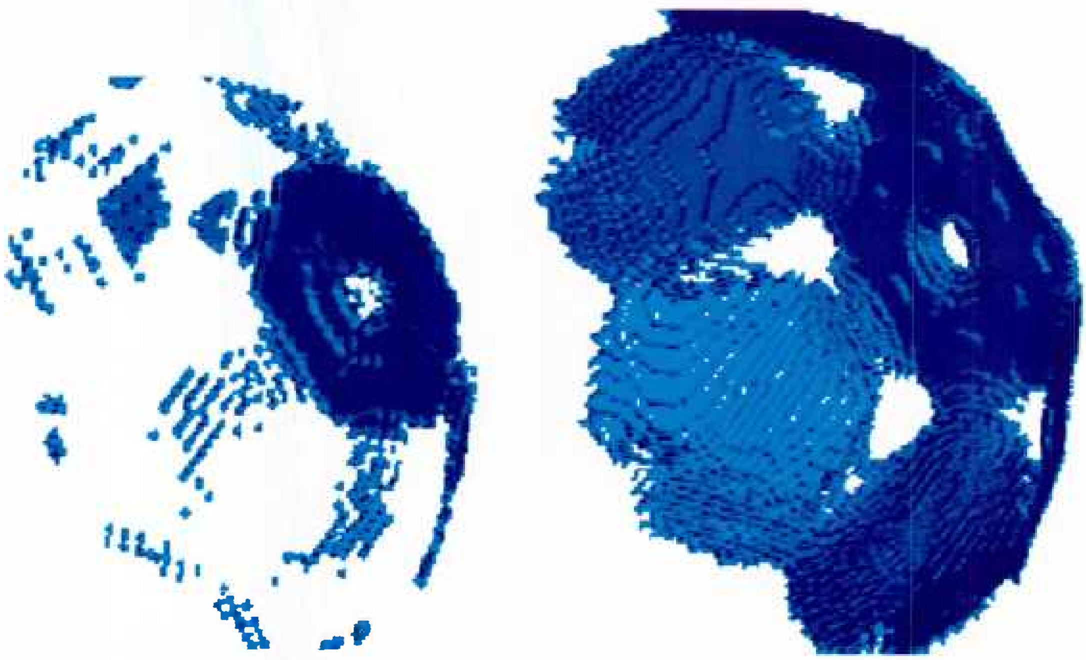
Computer Resource: TMC CM-5 [AHPCRC, Minneapolis, MN]

Research Objective: The ARDEC Energetics and Warheads Division is involved in the development of multimode anti-armor warheads. Modern explosively formed projectile warheads produce a single robust penetrating fragment. Greater lethality could often be achieved by a number of smaller fragments, depending on the target properties. The ARDEC Target Defeat Program is developing initiation-based multimode warheads to provide increased utility and overall lethality because of their applicability over a larger range of targets.

Methodology: Scalable computer technology is being investigated to solve multimode warhead design problems because of the limitations of CPU time and memory on current vector supercomputers. The computer program being used to do the modeling is PAGOSA, a Eulerian, scalable, high-rate, finite-difference program under development at Los Alamos National Laboratory.

Results: The problem illustrated is a seven-point rear initiation. Two mesh resolutions are shown. The 1-mm mesh is the largest problem that was able to be run on a Cray-2 (requiring 2 weeks CPU time). It was rerun on the CM-5 in 4 hours CPU time, but the mesh resolution was not fine enough to accurately represent the material properties. A 0.5-mm mesh run was made that used approximately 18 hours of CPU time on the CM-5. The modeling results are both visually and technically stunning. They clearly show physical behavior consistent with experimental results, which was not previously discernable [E.L. Baker and T.H. Vuong, "Massively Parallel Computation of Multimode Warhead Mechanics," 19th Army Science Conference, Orlando, FL, June 1994].

Significance: Using advanced, Eulerian, finite-difference modeling on scalable computers clearly shows a predictive capability of physical phenomena, which was not achievable with lower resolution modeling, successfully reproducing three initiation-mode experimental results. This constitutes a major step forward in modeling and design capability for multimode warhead development.



Seven-point rear initiation predicted liner configuration at 50 μs: (left) 1-mm meshing; (right) 0.5-mm meshing

Weapons Systems Safety Assessment: Structural Response to Aircraft Impacts

Tommy L. Bevins and Charles R. Malone
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

Computer Resource: Cray C-90 and Cray Y-MP [CEWES, Vicksburg, MS]

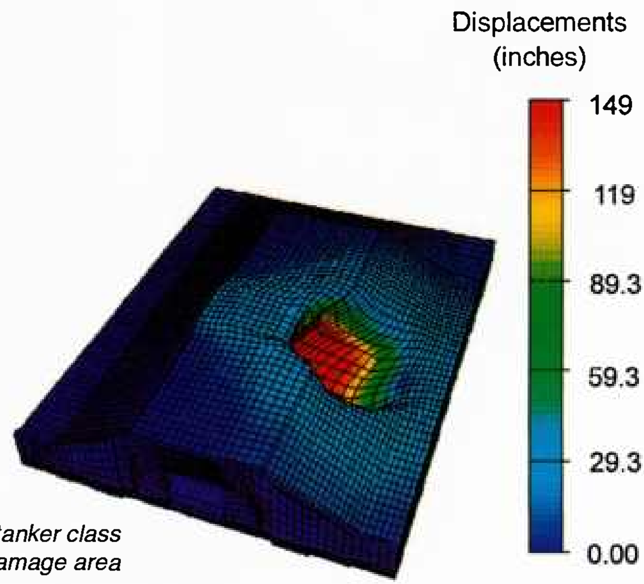
Research Objective: To determine the mass and velocity of fragments resulting from accidental aircraft impacts impinging on nuclear weapons storage containers. The mass and velocity information will then be used to assess the damage to the weapons containers and to determine if plutonium is released.

Methodology: A database of possible damage criteria for various aircraft crash scenarios was developed for a probability risk assessment. A core database was created using finite-element analysis on three structures, three different aircraft, three impact speeds, three azimuth angles, and three horizontal angles for a total of 243 required analyses. The analyses grids had approximately 170,000 degrees of freedom. The combination of grid size, the quantity of analyses, and nonlinear behavior required the use of both supercomputers at Waterways Experiment Station to meet project milestones. Approximately 1000 CPU hours were used over a period of 3 months to create the final database.

Results: The database of fragment mass and velocities was forwarded to other national laboratories to assess if the conditions would result in a plutonium release.

Significance: Results of this research, sponsored by the Defense Nuclear Agency, provided critical input to the Weapons System Safety Assessment Program for evaluating the probability of plutonium release resulting from accidental aircraft impact at nuclear weapon storage facilities.

Tanker class aircraft crashing into side of Igloo storage shelter



Finite-element results for tanker class aircraft showing damage area

Ship Structural Response to Underwater Explosions

Frederick A. Costanzo and George H. Camp, IV
Naval Surface Warfare Center, Portsmouth, VA

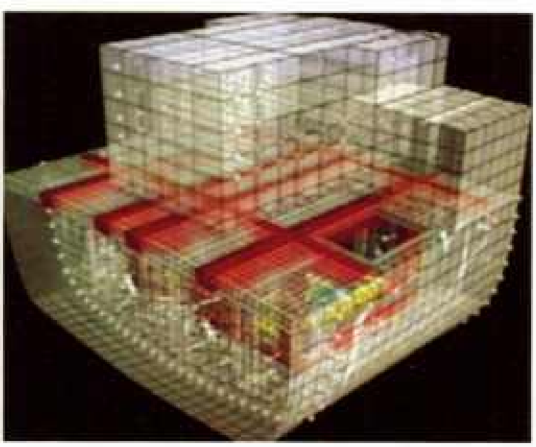
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To evaluate structural concepts critical to the survivability of ships, in particular coastal minehunters, which are subjected to underwater explosions.

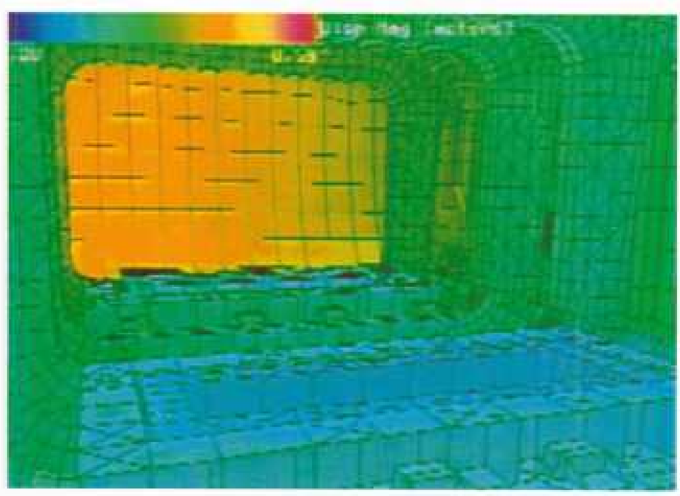
Methodology: A new class of coastal minehunter that must withstand a prescribed level of shock loading is being designed for use in littoral waters. This ship is to be constructed of glass-reinforced plastic and has a very complex arrangement in its equipment rooms. To assess designs for their ability to withstand such loads, transient shock analyses were performed for a variety of threat scenarios. The needed level of detail necessitated finite-element models for two main equipment rooms with a combined size of 200,000 degrees of freedom. This exceeded the capabilities of the NSWC Carderock Cray X-MP. It was determined that only the CEWES Cray C-90 could meet both the technical and programmatic requirements in the timeframe allowed.

Results: The shipbuilder had constructed a ship with a design that the analyses showed did not meet the specified shock requirements. These results, presented in the form of an animation video, were extremely critical for supporting negotiations with the shipbuilder, who concurred with the Navy's position that design-related problems existed and required correction.

Significance: The Navy views this work as an important success from several viewpoints. Based on high-performance computer predictions, a shipbuilder was required to acknowledge deficiencies. This was a major step toward ensuring the required design of a shock-hardened class of coastal minehunters. The Navy has gained great insight to the behavior of a complex composite structure subjected to underwater explosions, and new knowledge was gained in modeling methodologies for this type of problem.



Equipment room (through transparent hull)



Detailed contours of instantaneous displacements

Thermal/Stress Model of a Low Heat Rejection Diesel Head

Eugene Danielson
U.S. Army Tank Automotive Command, Warren, MI

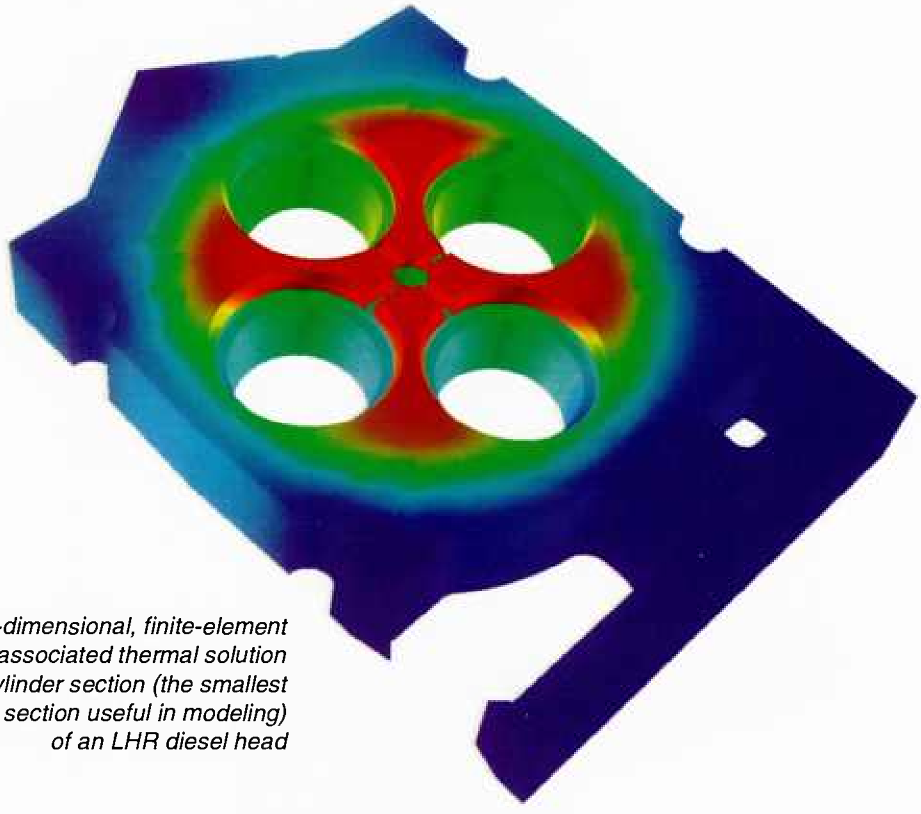
Computer Resource: Cray-2 [TACOM, Warren, MI]

Research Objective: To develop a model for thermal/stress analysis of low heat rejection (LHR) diesel components. The model is to be used to analytically characterize the thermal/stress fields, to determine the general magnitude of the stresses relative to material limits, and to conduct parametric material and design evaluations on LHR diesel heads. Very high radial compressive stresses can develop in these LHR heads as a result of constrained expansion of the high-temperature fire deck area inside the cylinder liner. Operational life is reduced unless care is taken in material selection and design.

Methodology: Computational requirements for this model/analysis are quite demanding. Thermal formulation (1 degree of freedom) required about 3 hours CPU time to solve; stress formulation (3 degrees of freedom) required about 7 hours CPU time to solve. Approximately 3.5 GB of memory (out of core) were needed for the stress solution. The basic model and each design variation contained about 41,000 elements and about 50,000 nodes. This size followed from a strict meshing criteria. Element aspect ratios were kept very low because of the complex geometry; element density was kept high because of high gradients (both thermal and stress) in the head.

Results: This modeling effort resulted in a material/design combination that potentially increases LHR head life.

Significance: Low heat rejection technology is an important cornerstone to the reduction in size and number of components for cooling and lubrication systems of diesel engines. In turn, this will provide diesel engines with greater reliability, lower fuel consumption, and lower maintenance and operation costs. In addition, the volume requiring armor protection will be reduced with consistent additional savings. Because this analysis was done on a generic head, any future diesel-powered fighting vehicle could benefit from LHR technology.



Three-dimensional, finite-element model and associated thermal solution of a one-cylinder section (the smallest symmetric section useful in modeling) of an LHR diesel head

Structural Acoustics of Double Hull Surface Ships

Gordon C. Everstine and Raymond S.-C. Cheng
Naval Surface Warfare Center, Bethesda, MD

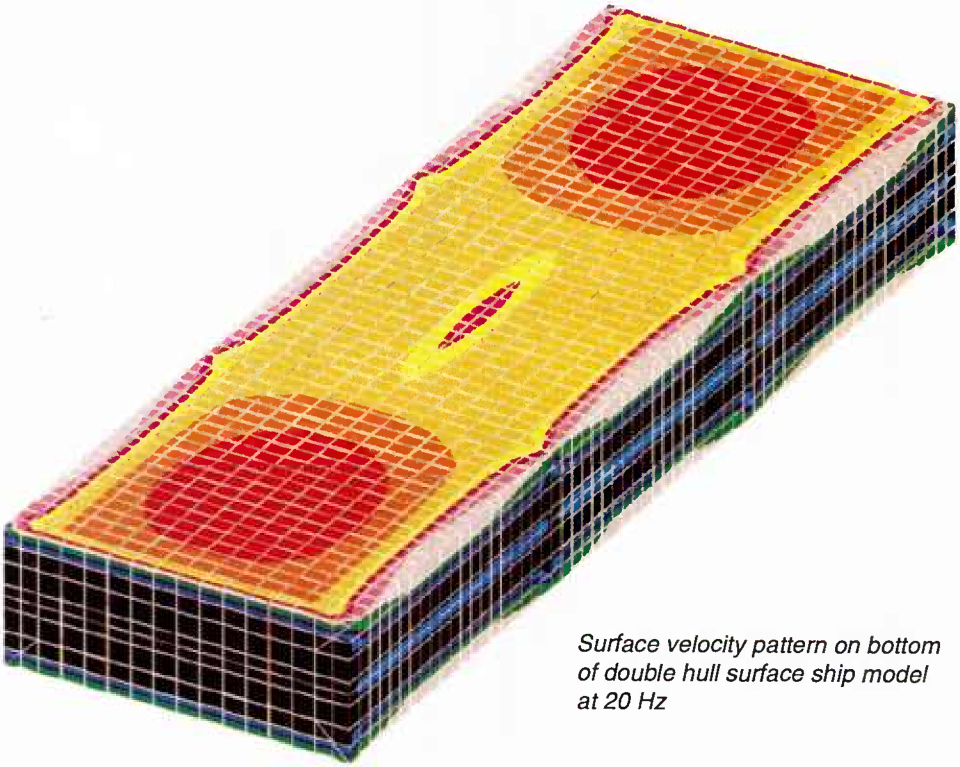
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: The Advanced Double Hull Technology Project seeks to fulfill the vision of an innovative surface ship concept to enhance the affordability, structural integrity, and survivability of both tankers and surface combatants. The double hull configuration can also be exploited for performance enhancements where stealth is desirable. The objectives of the acoustics investigations of the advanced double hull program were to determine the vibration and acoustic radiation characteristics of an advanced double hull configuration, to assess the capabilities of a compound coating to reduce radiated noise, and to demonstrate and validate large-scale computational tools for predicting the acoustic performance of double hull surface ships.

Methodology: The objectives were approached by using a coordinated blend of physical laboratory experiments and large-scale predictions on a computer model. The structural acoustic predictions used the structural analysis computer program NASTRAN and the structural acoustic program NASHUA. NASHUA uses a "first principles" approach to acoustic radiation and scattering prediction by coupling a boundary-element fluid model with a finite-element structural model. The approach requires detailed models of the actual geometry and results in many tens of thousands of coupled equations, necessitating the use of the fastest available high-performance computers.

Results: A compound coating installed in an advanced double hull model significantly reduced radiated noise as compared to an uncoated model in the "midfrequency" range. However, an uncoated double hull model appeared to offer no appreciable noise reduction compared to a single hull ship. The predictive model allows a variety of structural configurations to be assessed.

Significance: The findings are significant; they provide ship designers an additional avenue to noise control for Navy ships. It is estimated that these findings will avoid costs of approximately $0.5M per year by reducing the number of physical tests.



Surface velocity pattern on bottom of double hull surface ship model at 20 Hz

Structural-Acoustic Optimization Techniques

Stephen A. Hambric
Naval Surface Warfare Center, Bethesda, MD

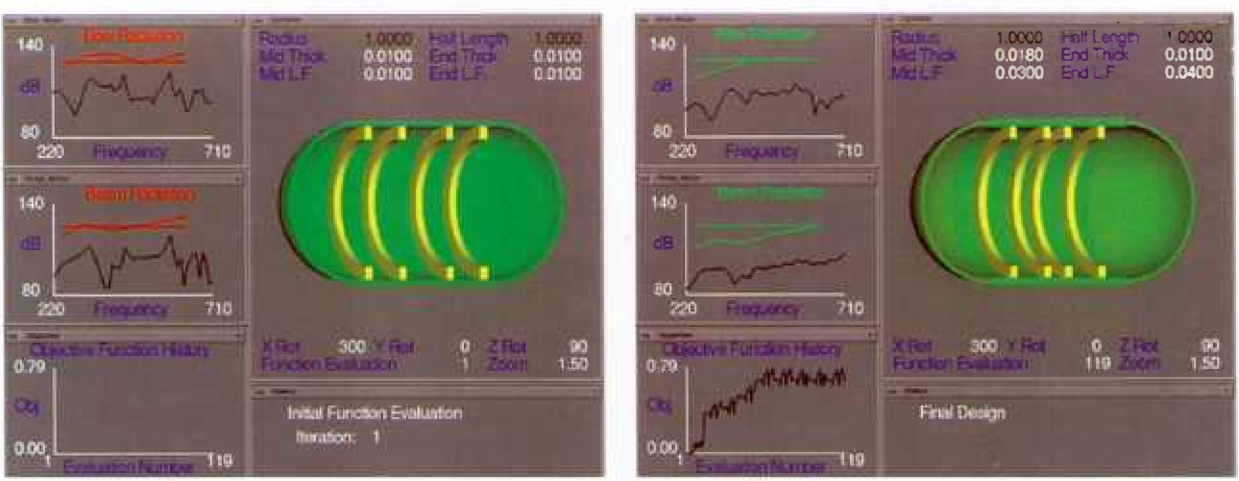
Computer Resource: Cray Y-MP [CEWES, Vicksburg, MS]

Research Objective: Noise control engineers are faced with the problem of reducing noise radiated from vibrating structures. Noise control techniques are applied based on engineering experience and can involve much trial and error. With the maturation of numerical structural vibration/acoustic radiation predictive methods, noise control designs can be tested by computational simulation of vibrating fluid structure systems. The research objective was therefore to derive accurate and efficient design synthesis methods to optimize the structural acoustic response of numerical models.

Methodology: Design optimization methods have been implemented in the computer program STRACOPT to automate the noise control design synthesis process. Search methods tailored specifically to structural acoustic optimization applications were derived to minimize structural weight while enforcing radiated-noise constraints. The algorithms automatically vary design parameters, such as material thicknesses and damping properties, and use the resulting response trends to determine an optimal design.

Results: STRACOPT was applied to finite-element models of several submerged cylindrical shell structures that were optimized to meet radiated-noise goal levels in the bow, beam, and stern directions. Global optimum designs were consistently found by STRACOPT from a wide range of initial design configurations [S.A. Hambric, "Approximation Techniques for Broadband Acoustic Radiated Noise Design Optimization Problems," presented at ASME Winter Annual Meeting, New Orleans, LA, 28 Nov. - 3 Dec. 1993].

Significance: The key benefit of this general methodology for weight and radiated-noise optimization is its applicability to reducing far-field radiated-noise signatures of submerged military vehicles. A secondary benefit of the optimization methodology is its applicability to a wider range of problems, including quieting of industrial machinery and reducing interior noise levels in automobiles and aircraft.



Initial and optimal designs of submerged, rib-stiffened, cylindrical shell structure

Structural Analysis of Bolted-on Propellers

Roger W. Hoffman and Robert D. Rockwell
Naval Surface Warfare Center, Bethesda, MD

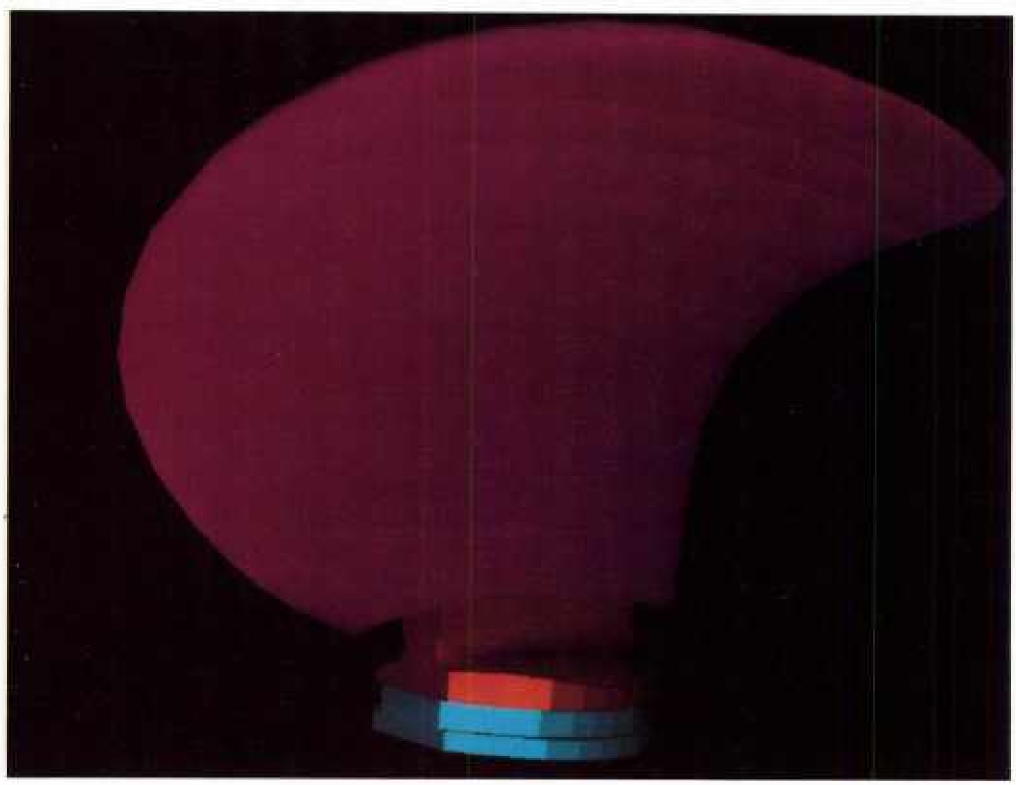
Computer Resource: Cray Y-MP [CEWES, Vicksburg, MS]

Research Objective: The purpose of the Quiet Surface Ship Advanced Technology Demonstration (ATD) Program is to transfer advanced surface ship propeller technology into systems development. A primary technology used in this program concerns the structural mechanics of bolted-on propeller blades. An important objective of the program was to determine the effects of blade geometry and loading on the structural response of blade bolts to certify propeller blades for at-sea service.

Methodology: The structural response of blade bolts was determined with both finite-element analysis and full-scale laboratory experiments. For the computer-aided computations, relevant structural components of a controllable pitch propeller system were represented using finite elements. Nonlinear contact finite-element analyses were executed to predict blade bolt structural response. This type of nonlinear analysis is extremely CPU intensive and required the resources available at CEWES.

Results: A three-dimensional, finite-element representation of a bolted-on propeller blade system was developed and was used to investigate the effect of blade geometry and loading on the structural response of propeller blade bolts. The analysis demonstrated that both bolt preload and blade-hub contact behavior have a significant impact on bolt response. Correlation of predicted bolt response with measured bolt response was high and established a basis for using this technology to certify U.S. Navy propeller blades for at-sea service.

Significance: Development of new structural analysis technology for propeller blades has increased our understanding of complex propeller blade attachment mechanics. This technology has been incorporated into the certification process for U.S. Navy bolted-on propeller blades for at-sea service.



Finite-element representation of surface ship propeller system

Analysis of 120-mm Tank Cannon Training Round

K. D. Kimsey
Army Research Laboratory, Aberdeen Proving Ground, MD

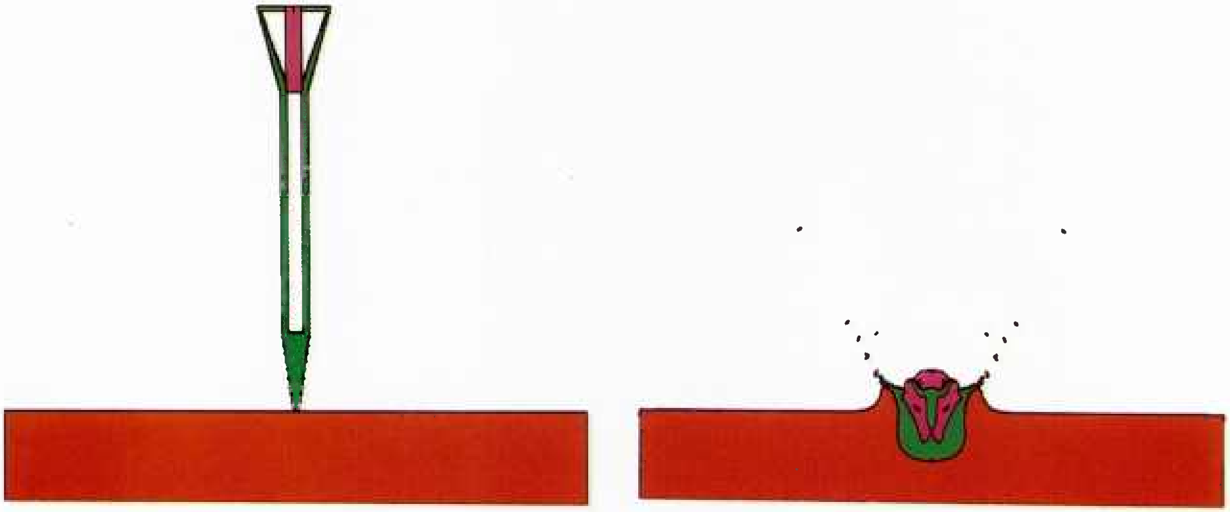
Computer Resource: Cray-2 [ARL, Aberdeen Proving Ground, MD]

Research Objective: Training ammunition is used to provide a realistic simulation of tank cannon ammunition in a controlled environment in terms of safety, range, and cost. The M865 is the current U.S. Army 120-mm kinetic energy projectile training ammunition. The steel core of the M865 has substantial potential for producing lethal damage in the event of a training accident. Researchers at the U.S. Army Research Laboratory recently conducted a combined computational and ballistic firing program to design and evaluate a 120-mm training round for mitigating lethal damage in the event of a training accident.

Methodology: Large-scale simulations were an integral part of the design and analysis of a hollow aluminum training round (HATR). Eulerian finite-difference simulations were used to model the HATR subjected to the high rate loading and large deformations encountered during impact.

Results: Performance of the HATR was measured in terms of depth of penetration into rolled homogeneous armor (RHA) at typical ordnance velocities. The HATR simulations predicted an order-of-magnitude reduction in penetration compared to the M865 over a broad range of striking velocities. The figure shows a typical HATR simulation at impact and at 340 µs after impact.

Significance: Ballistic firings and large-scale simulations have demonstrated a concept for reducing the potential lethal damage of large-caliber training ammunition by an order of magnitude. In addition, preliminary cost analyses estimate a 5% reduction in materials and manufacturing costs for the HATR compared to the M865. Considering the large quantity of tank cannon training ammunition procured each year by the U.S. Army, this represents a significant cost reduction.



Penetration of hollow aluminum training round: (left) T = 0 s ; (right) T = 340 µs

M1A1 Tank Lifting Eye Analysis

Stephen Lambrecht
U.S. Army Tank Automotive Command, Warren, MI

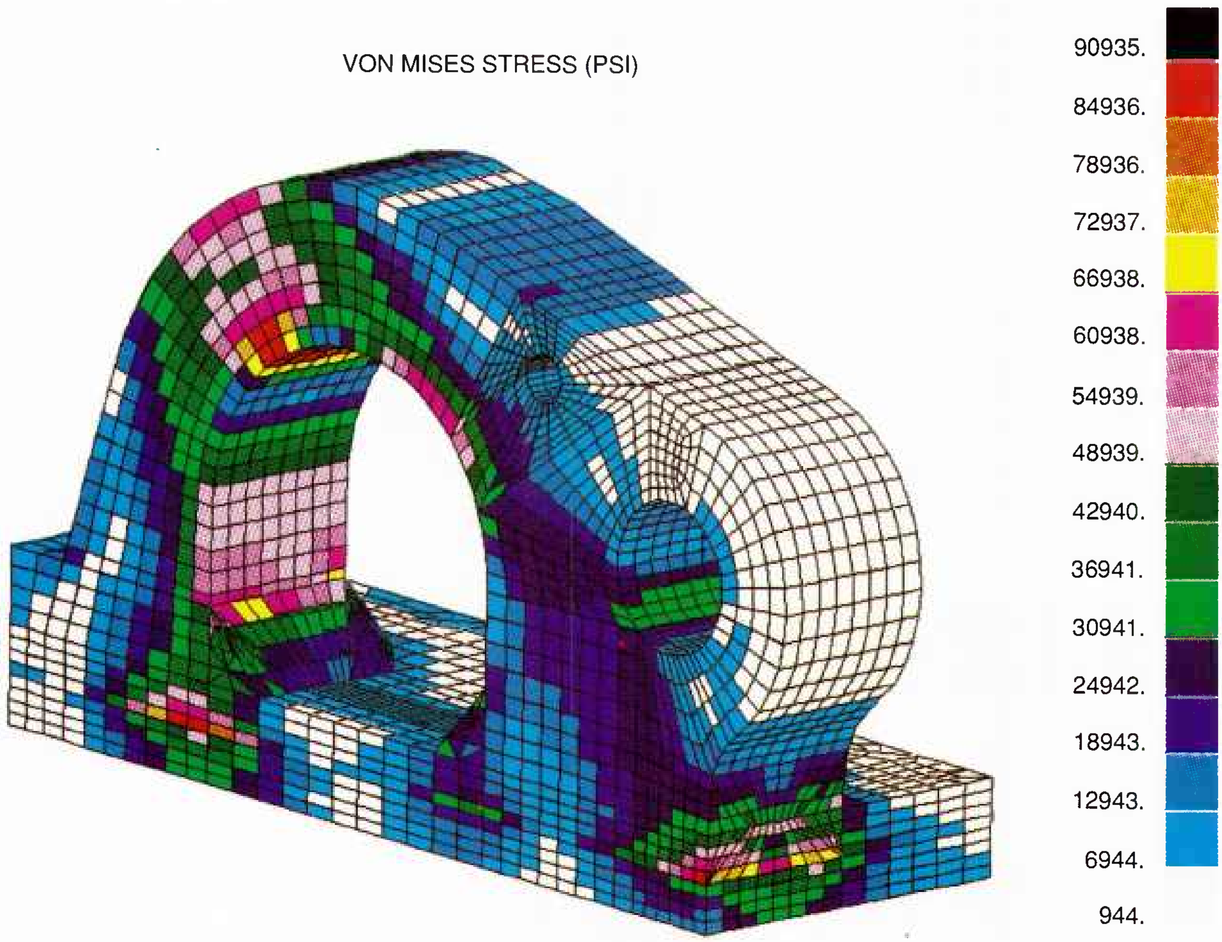
Computer Resource: Cray-2 [TACOM, Warren, MI]

Research Objective: Because of the increased weight of the M1A1 tank, a contractor-proposed redesign of the front lifting eye of the tank had to be analyzed. The redesign involved removing the old lifting eye and welding on a new, stronger one. Analyses were needed to determine the maximum strength of the lifting eye during overhead lifting operations and to find high stress areas.

Methodology: To evaluate the redesign, a three-dimensional, solid finite-element model of the M1A1 tank front lifting eye was created. Nonlinear finite-element analyses were performed on TARDEC's Cray-2 supercomputer using the ABAQUS code. A short 2-month turnaround was required to assure no slippage in the proposed redesign schedule if redesign were required.

Results: Twenty analyses were performed, using 120 hours of CPU time. The analyses showed that redesign was not necessary; only some welds needed to be added.

Significance: These analyses saved the U.S. Army $410,000 in tooling and materials, plus $350 in labor per vehicle that the redesign would have cost.



Finite-element mesh structure of the M1A1 lifting eye showing stress configurations

Structural Optimization of Concept Vehicles

Stephen Lambrecht
U.S. Army Tank Automotive Command, Warren, MI

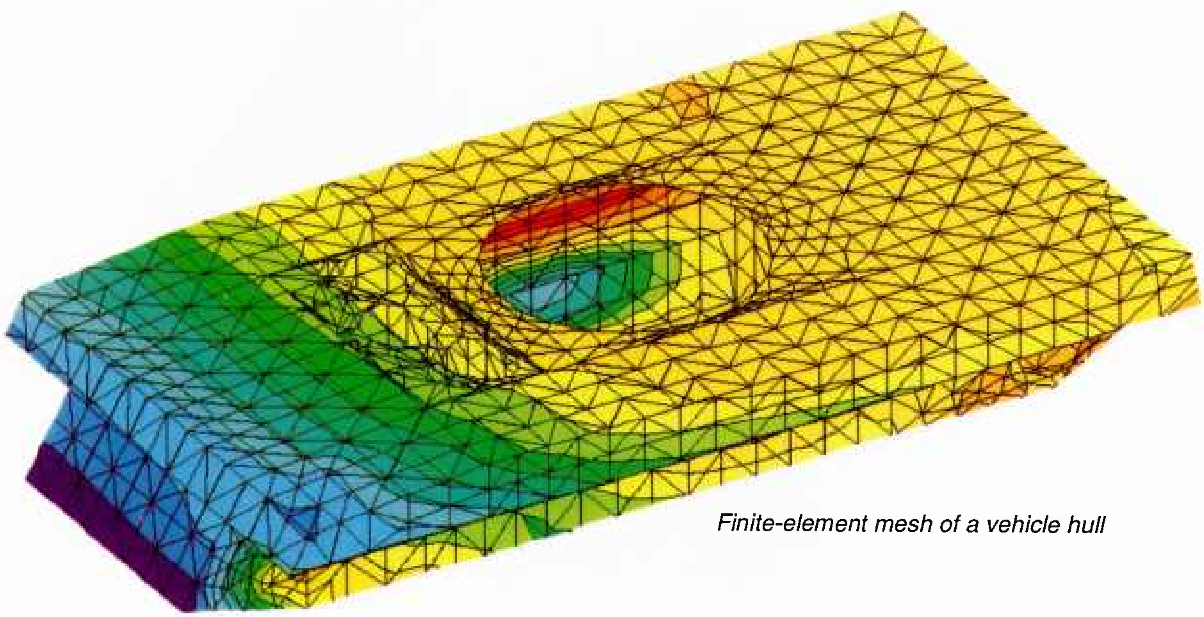
Computer Resource: Cray-2 [TACOM, Warren, MI]

Research Objective: In order to design the lightest vehicle hull, a structural optimization of several concept combat vehicle hulls is being performed. These analyses will optimize the structure only (no armor), for automotive, gun firing, towing, and lifting loads. This work is being performed to develop the lightest vehicle automotive structure that still has the integrity to support these loads.

Methodology: The design sensitivity analysis and optimization (DSO) tool is being used for this project. This structural design software system provides the designer with a graphics-based, menu-driven design environment to perform design sensitivity analysis and optimization for general sizing and shape design applications. The code allows the designer to evaluate how the size and shape design parameters, such as plate thickness or beam length, affect structural performance measures, which include stress, displacement, natural frequency, or weight. This capability combines commercial finite-element analysis codes such as PATRAN and ABAQUS with Center-developed DSO software. Finite-element models of the concept vehicle hull structures were constructed of three-node plate elements. Approximately 10 CPU hours are used for one optimization, and several optimizations are run for each vehicle.

Results: The weight of the first vehicle structure was reduced about 14,000 pounds, which is more than 10% of the vehicle weight. Approximately 100 CPU hours were used on TARDEC's Cray-2 supercomputer. A future optimization planned at the completion of this project is to look at the effect of reinforcing ribs on the structure. The DSO software system is an essential part of the virtual prototype loop, where a structure can be optimized to meet its particular mission before a prototype is built.

Significance: This preprototype optimization, showing a weight reduction of 10%, will save approximately 5 to 10% in material and tooling costs, thus reducing overall production costs of future vehicles.



Finite-element mesh of a vehicle hull

State-of-the-Art Standoff Demolition Techniques

Henry S. McDevitt, Jr.
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

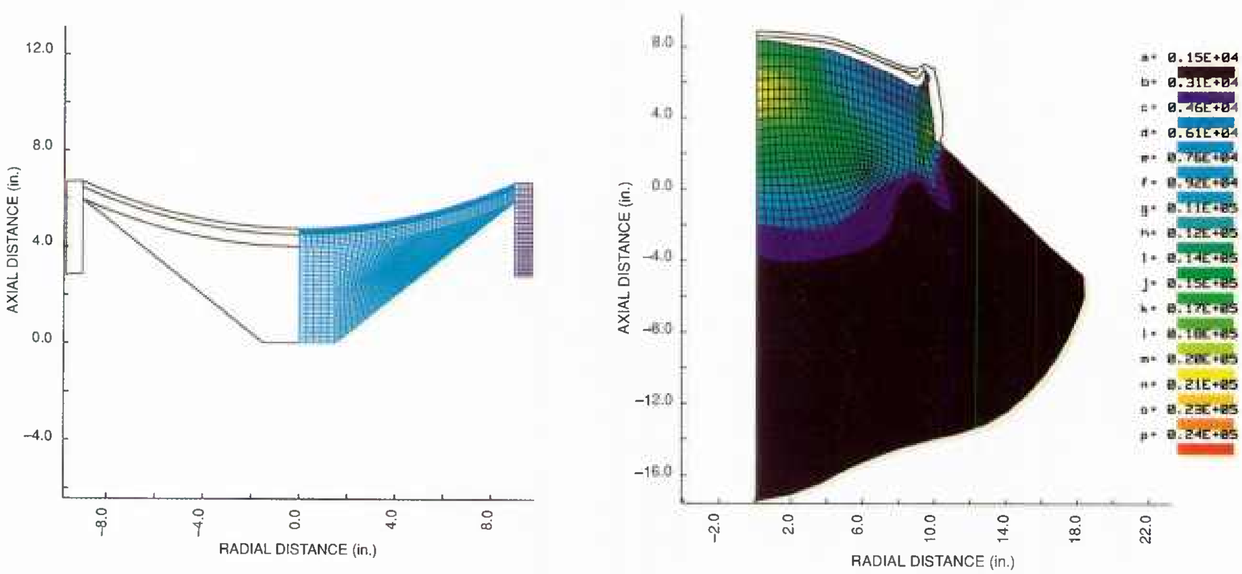
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To develop state-of-the-art standoff demolition techniques to support Combat Engineering and Special Operations mission requirements within the U.S. Army.

Methodology: Current demolition techniques expose troops to enemy fire and require excessive preparation times, manpower, and logistical support. Field experiments were conducted to establish the feasibility of the explosively formed penetrator (EFP) for standoff demolition applications. Parametric calculations were conducted on the Cray C-90 to optimize the shape of the explosive charge so that a cohesive slug would develop and provide maximum kinetic energy at the target. The final charge shape was verified through an intensive hydrodynamic calculation (50 CPU hours) that also verified earlier finite-element calculations on the slug formation and initial velocity.

Results: By using numerical models and field trials, the EFP has been developed into a new demolition munition that greatly enhances mission accomplishment while providing reduced risks to personnel. An explosive charge shaping apparatus, a key component of the EFP, was designed using the computational tools provided by the Cray C-90. This shaping apparatus was significant enough to earn a U.S. Patent (No. 5,323,681; dated 28 June 1994).

Significance: The EFP will provide combat engineer and special operations troops with a standoff demolition munition that is low-cost, simple, manportable, and has 2.5 times more destructive energy than a 155-mm artillery round. It has application for demolition missions against such targets as bridges, bunkers, and walls.



Simulation of EFP demolition munition: (left) Initial charge configuration; (right) Charge configuration and detonation pressure t = 80 µs

A Portable Parallel Smooth Particle Hydrodynamic Code Missile Defense Impact Simulation

Capt. Brad Smith, USAF, and Louis Baker
Phillips Laboratory, Kirtland AFB, NM

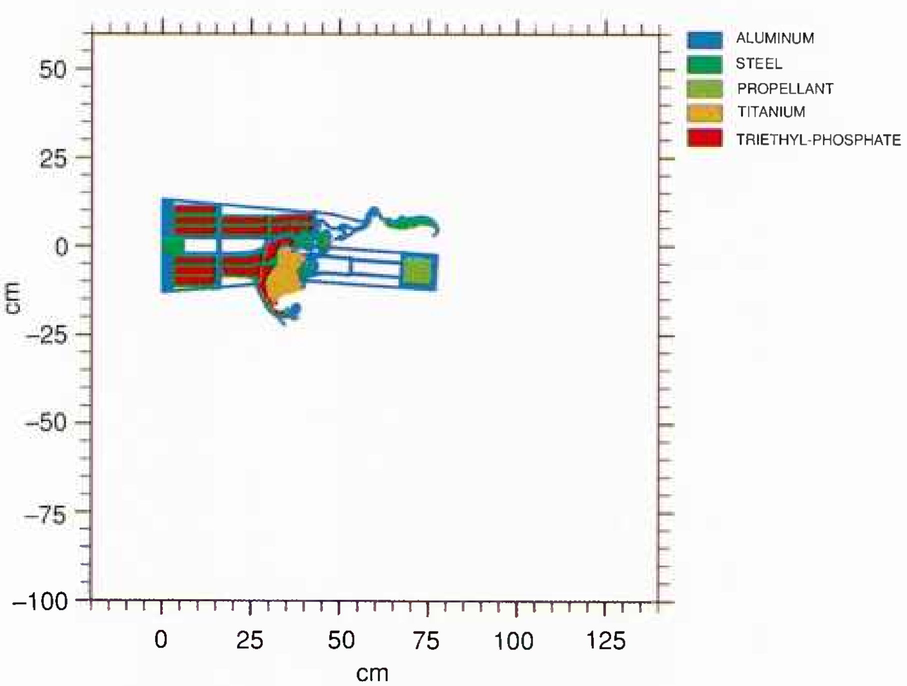
Computer Resource: IBM SP1 and SP2 [MHPCC, Kihei, HI]; Intel Paragon XP/S-15 [Wright-Patterson AFB, OH]; TMC CM-5E [NRL, Washington, DC]; and TMC CM-5 [AHPCRC, Minneapolis, MN]

Research Objective: To create a portable, parallel smooth particle hydrodynamic (PSPH) code that runs efficiently in parallel to reduce turnaround time for studies on kinetic weapon lethality, space environment, and survivability of manned and unmanned satellites. SPH is a first-principle, high-fidelity code for simulating the processes occurring during hypervelocity impacts and other high-energy interactions.

Methodology: PSPH is predicated on two previous SPH serial codes. The spatial decomposition of a problem is correlated to relative processor speeds to ensure good load balance. Processors are each allocated a portion of the problem in space, and they exchange border information at each time step. A weighted dynamic load balancing algorithm continually monitors the computational environment to minimize run time. A layered message passing library based on the message passing interface (MPI) standard over the parallel virtual machine (PVM) provides machine-independent message transport.

Results: A lethality study using PSPH for the Theater Missile Defense Program took less than 4 hours to run vs 2 days using old serial SPH codes. Similarly, a full satellite kinetic impact simulation for the Electronic Systems Command, previously viewed as impractical, was completed in less than a week. In a recent study for the Air Force Test and Evaluation Center, PSPH completed four simulations in a tenth of the time taken to run only two similar ones using serial methods. Through portability, reliance on any one DoD HPC asset has been eliminated.

Significance: The ability to respond more quickly and in greater detail has enhanced the survivability and lethality of space and missile systems. This measure of success enhances mission productivity of the Electronic Systems Command, the Air Force Test and Evaluation Center, the Ballistic Missile Defense Organization, and the Space Command.



Missile defense impact simulation; 300 μs

Computational Fluid Dynamics

Computational Fluid Dynamics is the accurate numerical solution of the equations describing fluid and gas motion. CFD is used for engineering design of DoD vehicles and propulsion systems as well as for basic studies of fluid dynamics and turbulence. It is therefore not surprising that CFD accounts for nearly half of the DoD's use of high performance computers.

The 32 CFD success stories that follow illustrate both grand challenge science and state-of-the-art engineering. The first 5 show applications at major Service laboratories of 5 different generic approaches to realistic CFD in very complex geometry. The next 11 describe research by some of the DoD's top academic and industrial contractors supported through ARO, AFOSR, ONR, and DNA sponsorship. The next 4 describe reactive flow and radiation transport CFD, coupling chemistry, ionization, and fluid dynamics. The final 12 contributions relate diverse Service-related applications including basic fluid dynamics studies, engineering design, Direct Simulation Monte Carlo, and magnetohydrodynamics.

Dr. Jay P. Boris
Naval Research Laboratory
CTA Leader for CFD

Tiltrotor Aerodynamics Using Scalable Software

Roger Strawn, Robert Meakin, Earl Duque, and W.J. McCroskey
Army Aeroflightdynamics Directorate (ATCOM), Moffett Field, CA

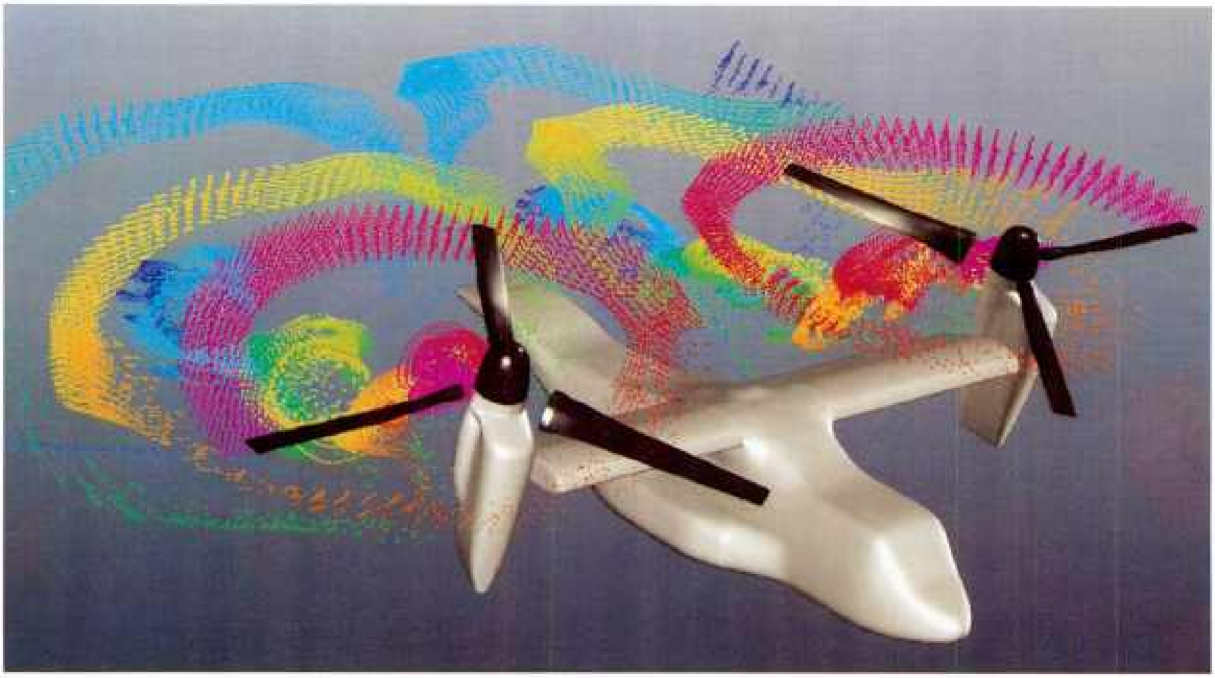
Computer Resource: Cray C-90 [NASA-Ames] and TMC CM-5 [AHPCRC, Minneapolis, MN]

Research Objective: To increase the mission effectiveness and reduce the noise, vibrations, and design cycle costs of future advanced rotorcraft. This requires validated faster and more reliable design and analysis codes for the aerodynamics and acoustics of complex rotorcraft configurations.

Methodology: Advanced computational fluid dynamics codes are being developed that exploit the advantages of an overset grid, or "Chimera," algorithm. This technique decomposes the aerodynamic flow field around a rotorcraft into a number of geometrically simple, overlapping grid zones associated with the various components. This is essential for treating the relative motion between the rotor blades and the airframe. The flow past each component is then computed using an efficient, implicit three-dimensional unsteady Navier-Stokes algorithm. Preliminary calculations on Cray C-90 and CM-5 supercomputers show that scalable parallel computing technology is essential for solving large problems such as complete rotorcraft.

Results: The aerodynamics of the V-22 tiltrotor aircraft have been simulated in flight conditions that had not been treated satisfactorily before (see figure). The results provide insight into the unsteady airloads and noise generated during landing and into the aircraft drag that limits high-speed cruise performance.

Significance: The ability to simulate accurately the aerodynamics and acoustics of rotorcraft will allow quieter and more efficient military and civilian vehicles to be designed at lower cost and less risk. Analysis of the computed flow separation on the airframe of the V-22 aircraft has already helped the manufacturers avoid costly redesign errors as they sought to improve the high-speed performance.



V-22 tiltrotor in helicopter mode forward flight; fight speed = 75 knots, Nacelle angle = 75°, and angle of attack = 5°

Ship Topside Airwakes for Safe Landing at Sea

Alexandra Landsberg, Theodore Young, Jr., Jay Boris,
William Sandberg, and Upul Obeysekare
Naval Research Laboratory, Washington, DC
Stephen Chun
Naval Sea Systems Command, Washington, DC

Computer Resource: Intel Paragon XP/S-15 [Wright-Patterson AFB, OH] and Intel iPSC/860 [NRL, Washington, DC]

Research Objective: To use the scalable FAST3D CFD models with the virtual cell embedding (VCE) grid generator to compute ship topside airwakes and to understand the turbulence environment caused by superstructure air vortex shedding to aid safe air vehicle landings at sea.

Methodology: FAST3D is a three-dimensional flow solver that incorporates the VCE method with the flux-corrected transport (FCT) algorithm. The most efficient implementations of CFD use a structured, orthogonal, rectilinear mesh, but complex bodies have had to be highly resolved to minimize the rough "staircasing" representation of the complex bodies. The VCE algorithm was developed to improve the accuracy around complex bodies without sacrificing CPU time or memory significantly. Parallel FAST3D with VCE is one of the DoD HPC benchmark codes.

Results: Complete production simulations for several minutes of real time are being performed. The air wake is extremely unsteady with energetic fluctuations from vortex shedding in the range that severely impacts helicopter dynamics. The coupled airwake/helicopter downwash calculation indicates that the downwash also significantly affects the unsteady airwake over the landing deck. These calculations have demonstrated that parallel FAST3D is a scalable code on the Paragon for this application. [See Landsberg, Young, Jr., and Boris, "An Efficient, Parallel Method for Solving Flows in Complex Geometries," AIAA Paper 94-0413 for details on the algorithms and the upcoming AIAA Paper 95-0047, "Analysis of the Nonlinear Coupling Effects of a Helicopter Downwash with an Unsteady Ship Airwake."]

Significance: This scalable production code is being used today to aid in the design and analysis of new naval surface combatants and to improve landing envelopes for safe air vehicle landings.

An instantaneous snapshot of the unsteady flow field around the DDG51 destroyer. The velocity vectors indicate the magnitude and sign of the flow around the superstructure. The temperature contours show 250° and 140° levels from the hot stack gases.

Two KC-135s in a Refueling Configuration

Capt. John Seo, USAF, and Stephen Scherr
Wright Laboratory, Wright-Patterson Air Force Base, OH

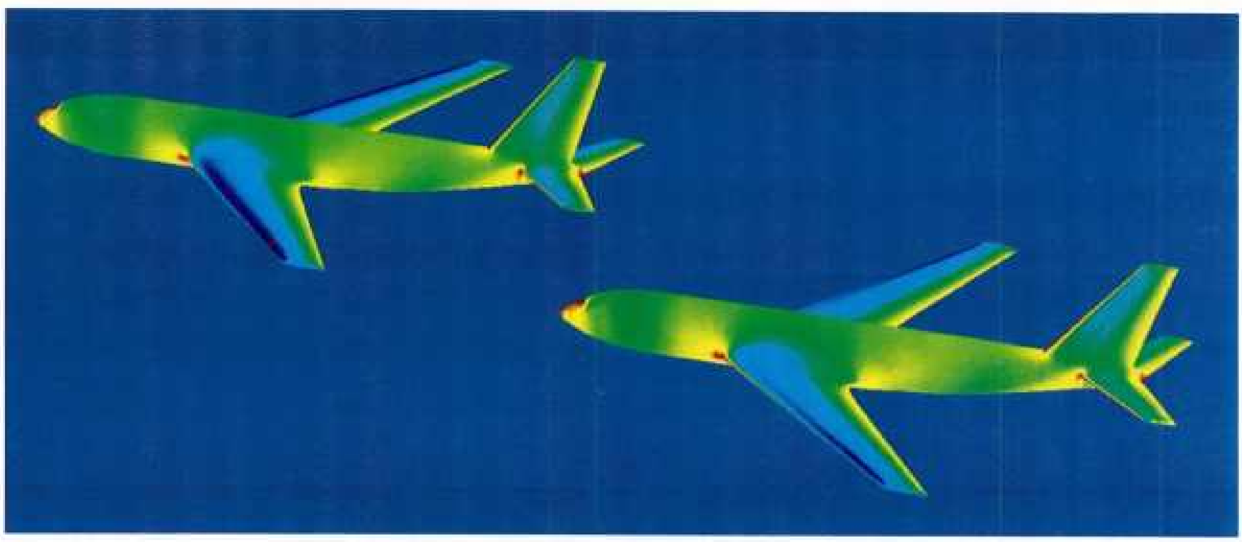
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]; IBM SP2 [MHPCC, Kihei, HI]; and Intel Paragon XP/S-15 [Wright-Patterson AFB, OH]

Research Objective: To develop improved understanding of the aerodynamics of refueling by calculating the airflow past two KC-135 aircraft at points during a refueling maneuver and to develop a portable, scalable, inviscid analysis code.

Methodology: The inviscid analysis code MERCURY is an explicit three-dimensional, arbitrary-body, fluid dynamics code developed in Wright Laboratory based on the techniques of Jameson. The code is parallelized by distributing grid blocks among processors and by using a portable message passing library. This approach requires only four types of changes and extends to similarly structured codes.

Results: Two different flow conditions were examined to assess the forces exerted on the two aircraft during a typical maneuver. The influence of the aircraft on each other agreed with flight test experience. Performance of the parallel code scaled linearly as the problem was refined, and calculations on the SP2 and Paragon were able to match the speed of the Cray as more processors were used ["Parallel MERCURY*:* Experiences with a Distributed Euler Solver," S.J. Scherr, OAI/OSC/NASA Symposium on Applications of Parallel and Distributed Computing, Columbus, OH, 18-19 April 1994].

Significance: This calculation was performed in support of Air Training Command. Further calculations will improve the ability of training simulations to model actual maneuver conditions and reduce flight test cost. Additionally, the parallel code increases the computational facilities available for solving problems in aircraft systems design. It enables more accurate and more complex analyses to be performed within cost and schedule constraints.



Surface pressure during KC-135 refueling maneuver; Mach = 0.3788, angle of attack = 2.6°

Torpedo Launch Dynamics

Ravi Ramamurti and William C. Sandberg
Naval Research Laboratory, Washington, DC
Rainald Löhner
George Mason University, Fairfax, VA
Office of Naval Research, Arlington, VA
J. Schwemin
Naval Undersea Warfare Center, Newport, RI

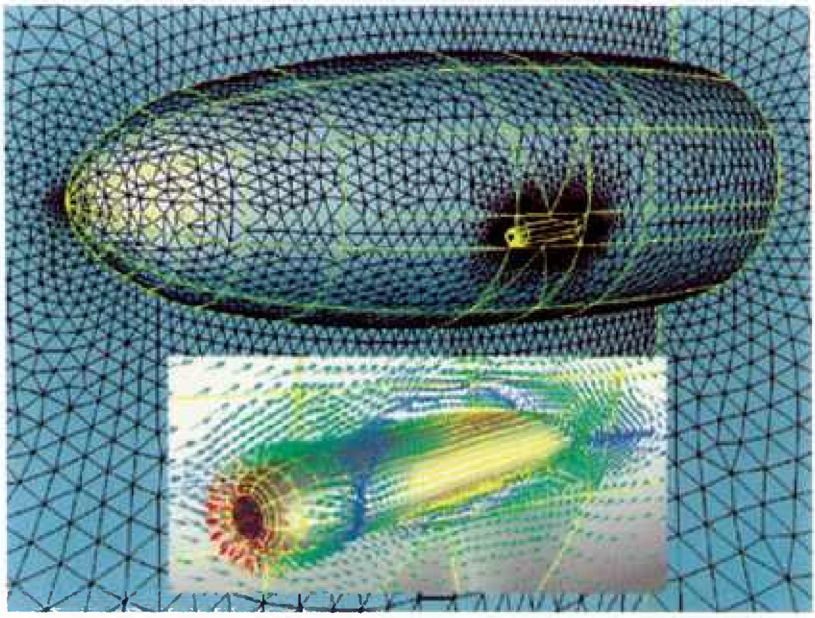
Computer Resource: Cray C-90 [NASA-Ames; CEWES, Vicksburg, MS]

Research Objective: To perform three-dimensional numerical simulations of the dynamics of the torpedo during the launch process from a submarine.

Methodology: An implicit finite-element solver, called FEFLOIC, for 3-D incompressible flows based on unstructured grids was used. The flow solver was parallelized for use with distributed memory computer architectures, and the scalability has been demonstrated using NRL CM-5 and Caltech Delta. This model is one of the DoD HPC benchmark codes. The flow solver was combined with adaptive remeshing techniques for transient problems with moving grids and was also integrated with the rigid body motion in a self-consistent manner, which allows the simulation of fully coupled fluid-rigid body interaction problems of arbitrary geometric complexity in three dimensions.

Results: The inviscid flow past a submarine and a torpedo during the launch process was simulated first using a grid comprising approximately 60,000 points and 280,000 tetrahedra and requiring approximately 60M words of memory. The forces and moments on the torpedo were obtained and compared with experiments. Improved adaptive remeshing techniques together with parallelization via autotasking reduced the wall clock time by a factor of 4.

Significance: This represents a new capability for computing launch dynamics and the trajectory of underwater weapons and vehicles of interest to the Navy. This code, in principle, can be applied to evaluate the low-speed, two-body trajectories for UUV launch and recovery.



Surface definition and velocity vectors during launch

Projectile with Wrap-around Fins

Harris L. Edge and Nisheeth Patel
U.S. Army Research Laboratory, Aberdeen Proving Ground, MD

Computer Resource: TMC CM-5 [AHPCRC, Minneapolis, MN] and Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To develop the ability to predict the roll moment coefficient for a projectile with wrap-around fins and to investigate the use of emerging massively parallel processor (MPP) computer architectures for production-type fluid flow applications.

Methodology: To design dynamically stable projectiles that have wrap-around fins requires the ability to predict the roll moment coefficient during the course of its trajectory. The unique aerodynamics of wrap-around fins are not completely understood, which makes analytical codes unreliable. Full Navier-Stokes computational fluid dynamics (CFD) computations that include viscous effects can provide an accurate model of the flow field upon which engineering designs can be based. CFD computations have reached a stage where a grid set involving several million points may be needed for complex geometrical shapes. For acceptable turnaround time, the computation requires a system with large memory and high performance. Because of hardware scalability and large in-core memory, MPP computers such as the CM-5 are becoming increasingly attractive for production-type CFD applications.

Results: Flow field solutions of a projectile with wrap-around fins have been computed for velocities ranging from Mach 1.3 to Mach 3.0. The roll moment coefficient computations have shown good agreement with experimental measurements. For an explicit, multizone, time-marching, full Navier-Stokes code along with a computational grid composed of approximately 1.5M points, performance of the CM-5 was found to be on par with that of the Cray C-90.

Significance: Results show that CFD can predict sensitive aerodynamic coefficients for complex missiles. Also, the CFD technique used is adaptable for other uses. The additional speed and memory of MPP computers will help in using CFD as a design tool to reduce design costs for both the military and private industry.

Pressure contours for a projectile with wrap-around fins

Tools for Improved Aerodynamic Design

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Virginia Polytechnic Institute and State University, Blacksburg, VA
Air Force Office of Scientific Research, Washington, DC

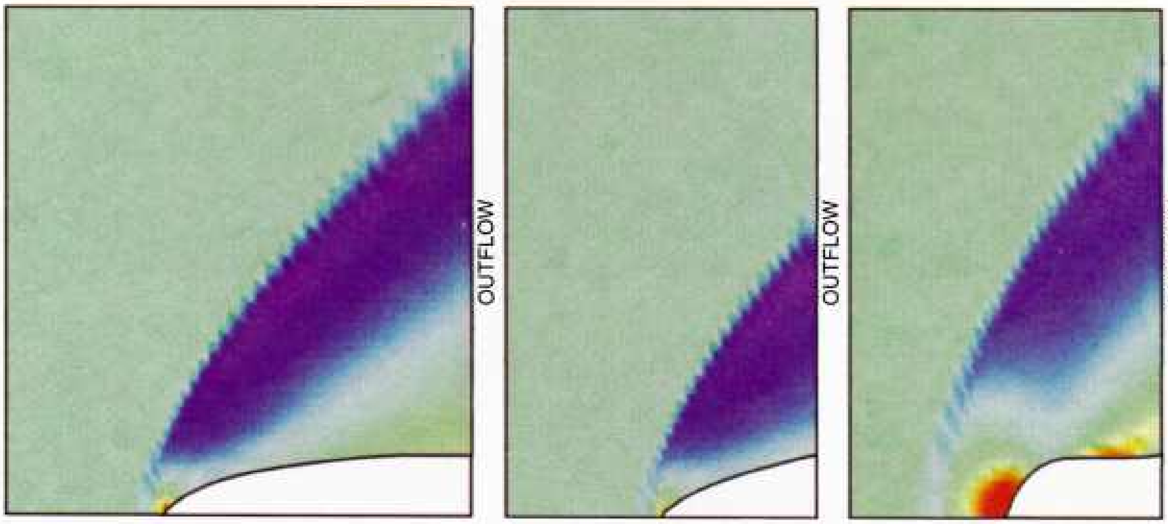
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To develop an efficient, parallel algorithm to model and analyze aerodynamic performance of an aerospace system in order to enhance performance by carefully tailoring shapes and fairings. Tools combining computational fluid dynamics (CFD) and optimization methods are valuable design aids that enhance performance and reduce development costs. Practical optimization schemes require information about the sensitivity of the flow to design changes, and efficient schemes to compute these sensitivities are extremely valuable.

Methodology: Standard finite-difference approximations are extremely costly in computational resources. As an alternative, we used the basic continuum model to derive sensitivity equations (SE), which are linear partial differential equations closely related to the underlying fluid dynamics. These were then solved in discrete approximation.

Results: An algorithm using this methodology was tested on a problem suggested by the design of the Free-Jet Test Facility at the Arnold Engineering Development Center (AEDC). The problem involved accurate simulation of the inlet flow for a jet engine. To account for effects of the forward fuselage, test engineers use a forebody simulator (FBS), which is necessarily more compact than the actual fuselage for geometric reasons. We considered a two-dimensional version of this optimal design problem. A target flow was produced by a long forebody, with the objective of achieving the best possible match to the outlet flow with a forebody that was one-half as long. The combined flow/sensitivity code was a modification of the PARC analysis code used at AEDC. The figure on the left shows the *x*-momentum for the long forebody (target flow), the center figure shows an initial estimate of the FBS, and the final figure shows the result after optimization using a Quasi-Newton/Trust-Region algorithm and gradient information from our SE method.

Significance: For a problem of modest size, timing tests show that the SE method produces 50% savings in computer time. More importantly, the method lends itself to parallel implementation; for large problems, the savings will be 90% or more. Consequently, this new algorithm can be used to attack practical three-dimensional aerodynamic design problems that were, until now, not computationally feasible.



Long forebody target flow   *Short forebody initial estimate*   *Short forebody optimal shape*

Supersonic Compressible Turbulence

Linda D. Kral and John F. Donovan
McDonnell Douglas Corporation, St. Louis, MO
Air Force Office of Scientific Research, Washington, DC

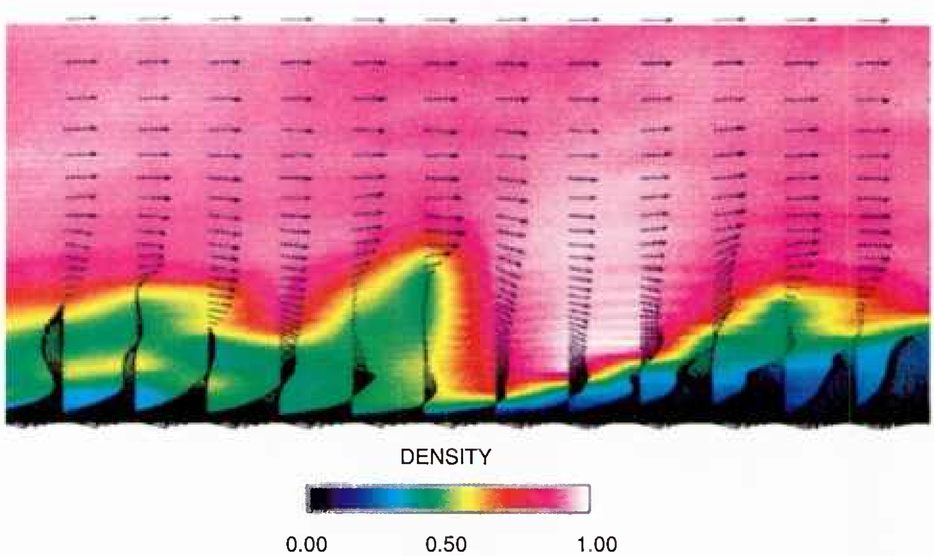
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To extend the understanding of compressible turbulence by modeling the turbulence structure of compressible, transitional, and turbulent flows over complex flight vehicle geometries by large eddy simulation (LES).

Methodology: The Favre-filtered, compressible, three-dimensional Navier-Stokes equations are solved in conservative form using generalized coordinates. The large scales of motion are resolved and the small scales are modeled. Sixth-order compact differences are used for the spatial discretization, and a third-order Runge-Kutta scheme is used for the time advancement. The numerical algorithm is fully vectorized on the Cray C-90. This research could not have been possible without the use of the C-90.

Results: Smagorinsky and structure function subgrid models have been tested in the LES simulation. The first LES simulation of supersonic wall-bounded flow has been accomplished. The figure shows velocity vectors superimposed on density contours in the supersonic (Mach 4.5) boundary layer over a flat plate. The turbulence structures are convecting at 0.85 times the free stream velocity. Low density fluid is lifted up from the wall, and local shear layers are observed away from the wall that are associated with low-density turbulence structures. The downstream "bulge" is in the early stages of development as depicted by the strong shear layers seen on the upstream side.

Significance: Our ability to design commercial and military aircraft is severely hindered by a total lack of understanding of the behavior of compressible turbulence structures in the transitional as well as fully turbulent flows over these aircraft. At present, all design calculations are based on turbulence models, which themselves use fully empirical models of turbulence based on mean flow properties. Only LES methods are capable of simulating the detailed structure and properties of turbulence. This will lead to increased range, payload, and performance for military aircraft and increased range at greatly reduced fuel consumption for commercial aircraft.



Compressible turbulence structure on a flat plate

Compressible Turbulence

Doyle D. Knight
Rutgers University, New Brunswick, NJ
Air Force Office of Scientific Research, Washington, DC

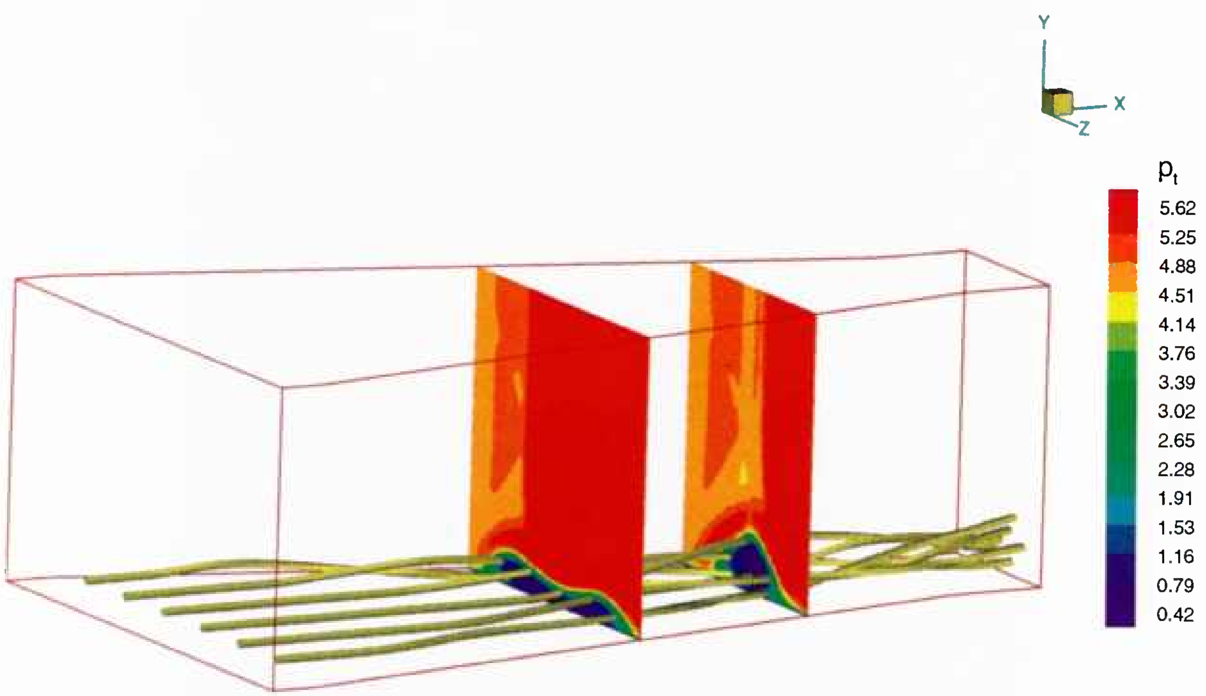
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To improve the fundamental understanding of complex viscous-inviscid interaction flowfields of crossing shock-wave/turbulent boundary layer interactions that arise in supersonic and hypersonic air-breathing engine inlets at yaw.

Methodology: The three-dimensional Reynolds-averaged compressible Navier-Stokes equations are solved in strong conservation law form by using a body-fitted coordinate transformation and a two-equation turbulence model. The numerical algorithm uses a flux-difference split technique for the inviscid fluxes and central differencing for the viscous and heat transfer terms. The algorithm is highly vectorized on the Cray C-90. This research would not have been possible without the use of the C-90.

Results: Results have been obtained for Mach 3.85 flows and asymmetric inlet ramp configurations of 7/11 and 11/15 degrees. Incoming flow streamlines are shown to quickly coalesce and roll up in braided fashion along the inlet centerline. The computed flowfield describes the complex reflected shock patterns and formation of counterrotating asymmetric vortices. This roll-up produces a concentrated region of high inlet distortion resulting in significant loss of thrust.

Significance: This research has revealed the fundamental nature of high-speed (supersonic and hypersonic) air-breathing engine inlet flows at yaw. This will lead to military as well as commercial air-breathing engine inlets that will provide increased thrust and performance.



Shock-wave/turbulent boundary layer interaction streamlines

Largest Simulation of Homogeneous Compressible Turbulence

David H. Porter, Paul Woodward, and Steven Anderson
Army High Performance Computing Research Center, Minneapolis, MN
Army Research Office, RTP, NC

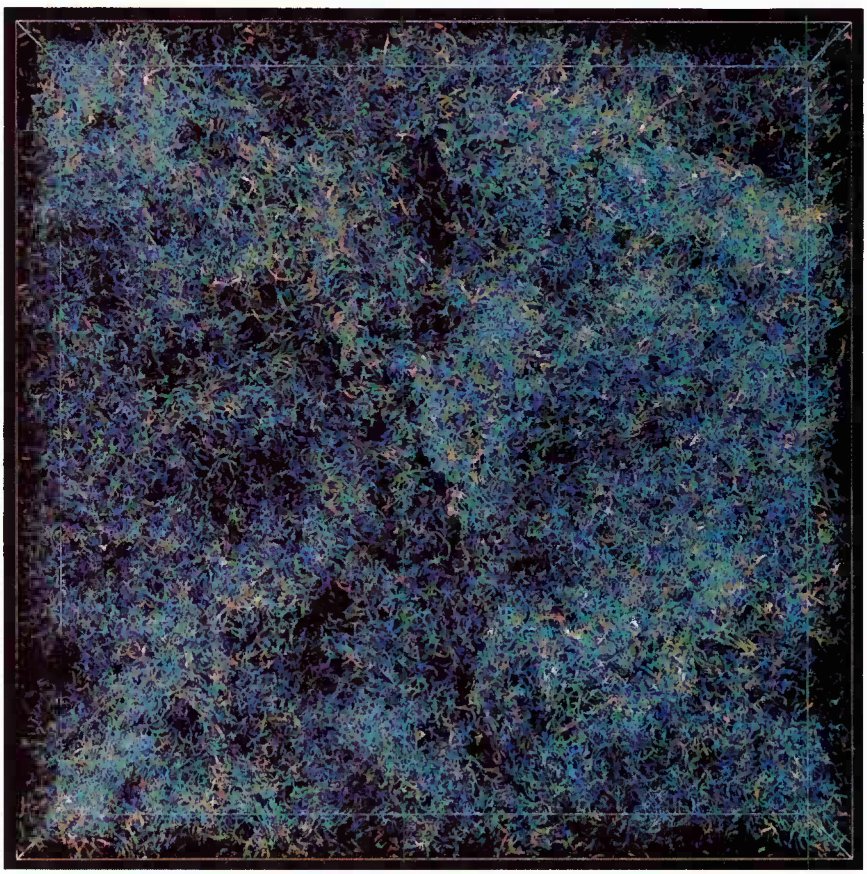
Computer Resource: A prototype "Challenge Array" built by Silicon Graphics for this computation.

Research Objective: To simulate homogeneous, compressible turbulence in sufficient detail to test competing theoretical statistical models of turbulence.

Methodology: The parallelized PPM code developed originally for the Connection Machine was adapted to run on a cluster of 16 silicon graphics workstations, each with 20 MIPS R-4400 (100 MHz) processors and 1.75 GB of memory and each interconnected by 20 FDDI rings. The 28 GB system memory was critical in enabling this grand challenge computation, which ran at 4.9 Gflops. The 500 GB data set from this run will be compared with predictions of turbulence closure models. The PPM gas dynamics code was parallelized and optimized for this experimental hardware configuration and was run using a grid of 1024 x 1024 x 1024 cells.

Results: This simulation, a joint University of Minnesota AHPCRC and Silicon Graphics project, is the largest turbulence simulation to date, producing 500 GB of data for analysis and visualization in the Graphics and Visualization Laboratory of the AHPCRC.

Significance: The phenomenon of compressible fluid turbulence is fundamental to engineering of aerodynamic, hydrodynamic, and ballistic systems, both for the DoD and the commercial sector.



PPM simulation of homogeneous, compressible turbulence on a 1024 x 1024 x 1024 grid

Large Ram Air Parachutes

S.K. Aliabadi, W. Garrard, V. Kalro, S. Mittal, and T.E. Tezduyar
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Army Research Office, RTP, NC
K. Stein
Natick Research, Development, and Engineering Center, Natick MA

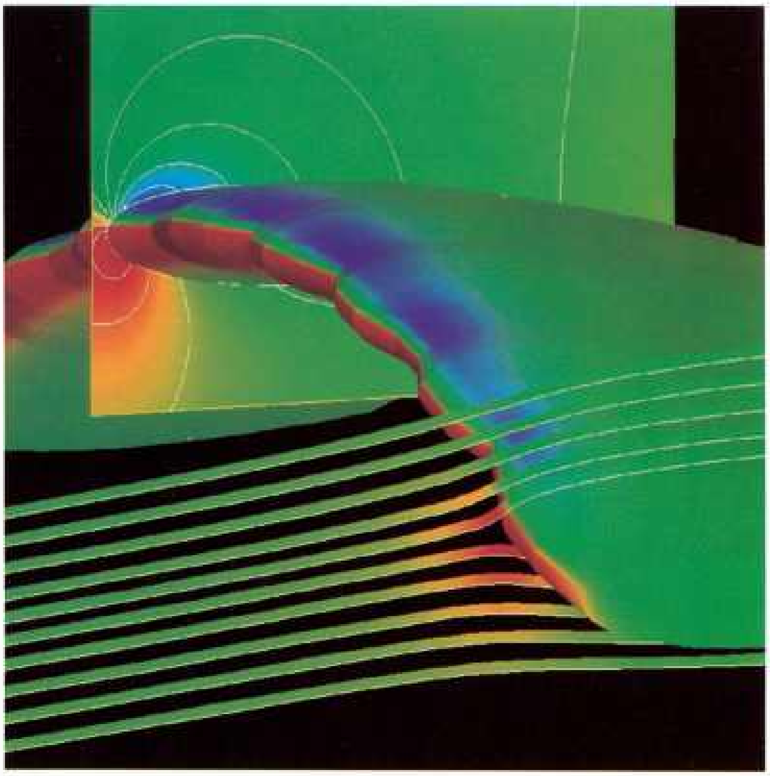
Computer Resource: TMC CM-5 [AHPCRC, Minneapolis, MN]

Research Objective: To develop techniques that accurately predict the performance and dynamics of large parafoils, from inflation to full deployment. Parafoils have been widely used by the sport parachute community and are finding increasing application in the deployment of large payloads, such as spacecraft, ground vehicles, and large emergency food and supplies crates.

Methodology: A stabilized finite-element formulation of full Navier-Stokes equations governing flows of incompressible fluids has been implemented on the CM-5. A simple turbulence model accounts for the Reynolds stresses in the turbulent flow. More than 370,000 hexahedral elements are in the mesh; more than 1,460,000 equations are solved simultaneously at each nonlinear iteration.

Results: Flow past a large ram air parachute during a steady gliding descent at Reynolds number 10 million is simulated. Steady-state computations were performed at 5°, 10°, and 15° angles of attack. Aerodynamic coefficients and lift/drag ratios obtained from the computations are in good agreement with experimental data.

Significance: The parallel implementation allows problems with more degrees of freedom to be solved with greater accuracy than has previously been possible. The results of these simulations are being applied to the deployment of safer and larger ram air parachutes for military, commercial, sports, space, and relief applications.



Pressure distribution on the parafoil surface and a spanwise cross section, and a set of stream ribbons color-coded with the pressure.

Finite-Element Methodologies for Advanced Injector Design

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U.S. Army Research Laboratory, Aberdeen Proving Ground, MD
S. E. Ray and T. E. Tezduyar
Army High Performance Computing Research Center, Minneapolis, MN
Army Research Office, RTP, NC

Computer Resource: Cray C-90 [AHPCRC, Minneapolis, MN]

Research Objective: To improve the design of the injector in the regenerative liquid propellant gun (RLPG) through the use of state-of-the-art finite-element methods. The injector region is an annular orifice formed by two axisymmetric pistons that move rearward during the firing cycle.

Methodology: By applying a predetermined pressure history on the combustion chamber side of the injector region of the RLPG, researchers at ARL and at the prime U.S. contractor for the RLPG armament system evaluated the potential for flow reversal in various injector designs.

Results: Applying these methods to the design process has helped researchers to understand the injection process. Preliminary results have indicated that this tool can be used to evaluate injector designs based on the potential for flow reversal of the injector.

Significance: The development of a proper injector design is critical to the success of the armament system for the Advanced Field Artillery System/Future Armored Resupply Vehicle (AFAS/FARV). The methods used are relevant to the design of injectors in other applications such as internal combustion engines.

Propagation of a pressure wave toward the injector

Fuel-Air Mixing Enhanced by Shock-induced Vortices

David Gottlieb, Wai-Sun Don, Chi-Wang Shu, and Carl Quillen
Brown University, Providence, RI
Air Force Office of Scientific Research, Washington, DC

Computer Resource: Cray C-90 [CEWES, Vicksburg, MS] and TMC CM-5 [AHPCRC, Minneapolis, MN]

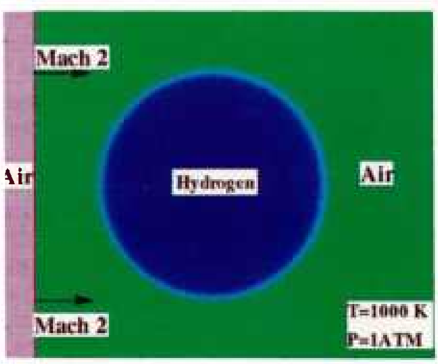
Research Objective: To study the possibility of enhancing combustion efficiency by using the interaction of a shock wave and a hydrogen jet. This is relevant for the design of air-breathing scramjet engines; it may provide a mechanism for inducing millisecond combustion times.

Methodology: The full Navier-Stokes equations governing the fuel-air transport, with additional equations for the conservation of mass of the reactants and products of combustion, were numerically solved. To obtain meaningful information about the combustion process, high-order numerical schemes were used. These are pseudospectral shock-capturing methods and high-order, finite-difference, essentially nonoscillatory (ENO) schemes. The ENO scheme, which is prohibitively slow on the serial machines, was implemented via domain decomposition on the CM-5 parallel supercomputer. The computational kernel was coded in low-level assembly language and achieved performance in excess of 1 Gflop on 32 nodes, with parallel efficiencies in excess of 95% for problem sizes as small as 500^2 points. The spectral code was based on the Chebyshev collocation method.

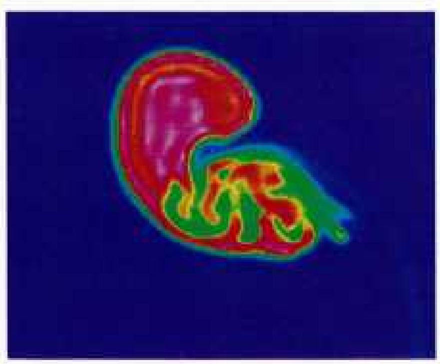
Results: The computational kernel of the algorithm achieved performance of 600 Mflops on a single-processor Cray C-90. The figure shows the hydrogen mass fraction of the fuel-air mixture after passage of the shock. The importance of high resolution in resolving the combustion process is evident from the lack of structure in (b). Results obtained show detailed structure of the jet after interacting with the shock.

Significance: High-order methods such as those developed here are critical to adequately quantify the shock-enhanced vortical mixing in scramjets. The codes described will be extremely useful in future optimal design of air-breathing scramjet engines for use in the National Aerospace Plane and in high-speed civilian transport.

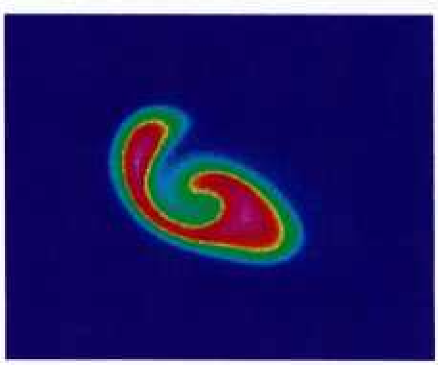
(a) Initial density condition



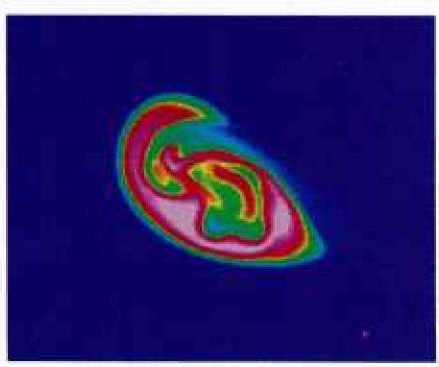
(b) Spectral method, 60 µs (400 x 320)



(c) Low-resolution ENO, 60 µs (240 x 120)



(d) High-resolution ENO, 60 µs (752 x 376)



Hydrogen mass fraction

Scattering and Dissipation of Waves by Turbulence

Douglas G. Dommermuth and Rebecca C.Y. Mui
Science Applications International Corporation, San Diego, CA
Office of Naval Research, Arlington, VA

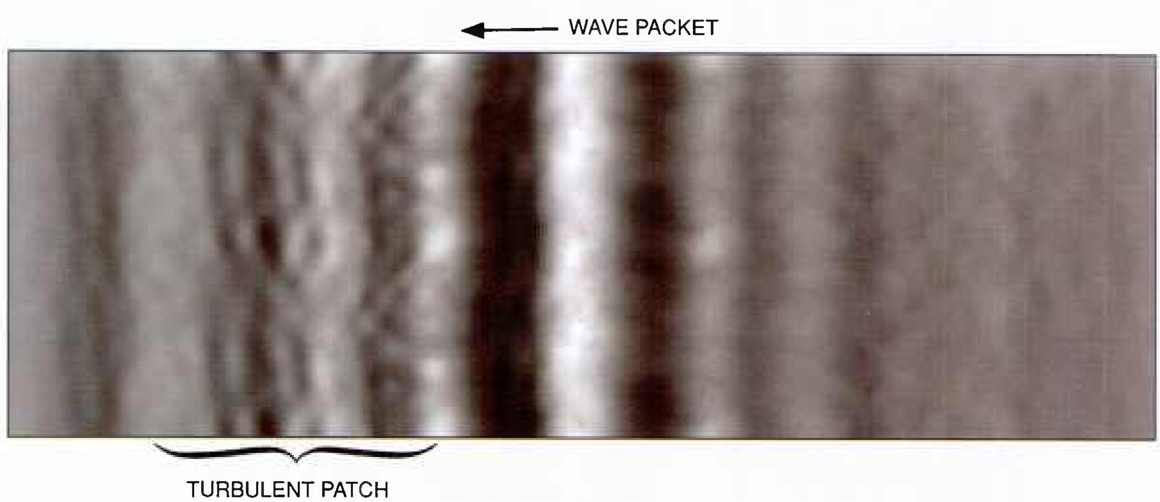
Computer Resource: TMC CM-5 [NRL, Washington, DC; AHPCRC, Minneapolis, MN]

Research Objective: We are developing capabilities to understand and model the turbulent scattering and dissipation of free-surface waves. The major goal of our research is to quantify how free-surface turbulence affects the remote sensing of ship wakes. The results of the research will benefit a DoD ship-wake program whose major focus is the detection of ship wakes. The results of the research will also ultimately improve our understanding of post-breaking waves, air entrainment, bubbly flow, and the transfer of heat, wind energy, momentum, and gases at the air/water interface.

Methodology: Direct numerical simulations of surface waves have been performed to investigate roughening of the surface and scattering of waves by turbulence. The simulations use a finite-difference code that has been optimized to perform on a CM-5 computer.

Results: Two wave-induced coherent vortical structures form at the edges of the patch of turbulence. The formation of these vortical structures may help to explain the observed persistence of ship wakes and the spreading of surfactants to the edges of a ship wake. In the near field of a ship, hull shaping and vortex generators may be used to generate large vortical structures to break up the windward and leeward vortices that form at the edges of a ship wake. As a result, we may be able to reduce the signature of a ship as viewed by various remote sensing devices [D.G. Dommermuth, E.A. Novikov, and R.C.Y. Mui, "The Interaction of Surface Waves with Turbulence," in *Proceedings of the Symposium on Free-Surface Turbulence*, Lake Tahoe (1994), to appear].

Significance: The results of our investigation of surface waves interacting with a patch of turbulence suggest a new technique to control turbulent boundary layers. By inducing undulations in the walls of vehicles, we hope to duplicate the effects of free-surface waves. Potential applications of boundary-layer control that are relevant to Navy interests include drag reduction for pipe flows and vehicles. Aside from drag reduction, the ability to organize turbulence could have numerous applications in both Navy and civilian sectors, such as fuel efficiency and pollution control.



Turbulent scattering

Initial Stages of a Microbreaking Wave

Douglas G. Dommermuth and Rebecca C.Y. Mui
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Office of Naval Research, Arlington, VA

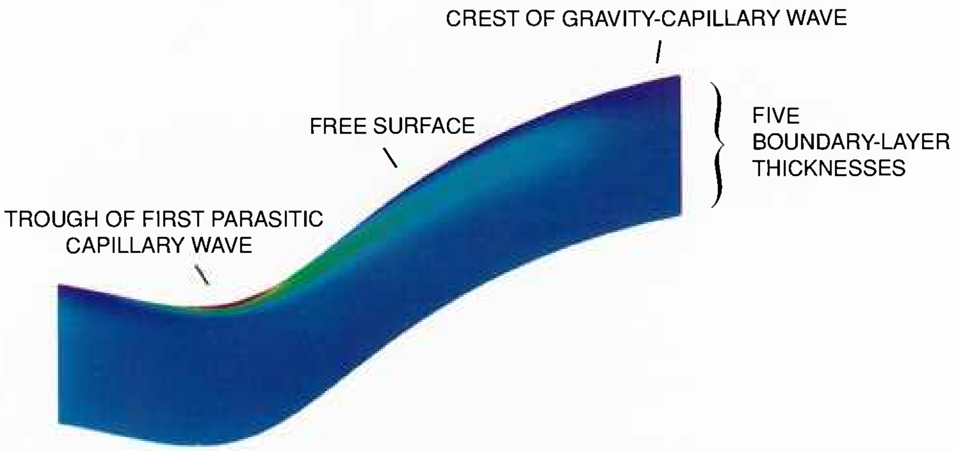
Computer Resource: TMC CM-5 [NRL, Washington, DC; AHPCRC, Minneapolis, MN]

Research Objective: We are studying short-scale waves to help isolate man-made disturbances from natural disturbances in remotely sensed images of the ocean surface. The results of our research benefit a DoD ship-wake program whose major focus is the detection of ship wakes.

Methodology: We are performing numerical simulations of the early stages of small breaking waves with 5- to 10-cm wavelengths. We have developed a unique, flexible, and accurate numerical algorithm, which we call Taylor's Accurate Method of Evaluation (TAME). This algorithm uses the capabilities of the CM-5 computer to solve very complex initial-boundary-value problems and combines the best features of finite-difference, finite-volume, and finite-element techniques. We believe that the TAME algorithm will become the method of choice for solving complex boundary conditions with complex geometries. Parallel computers such as the CM-5 are the only practical platforms that are capable of implementing the TAME algorithm.

Results: An investigation of a microbreaking wave has been completed. A thin vortical layer separates near the crest of the wave. The layer is so thin and convoluted that laboratory techniques may never be able to measure it. Yet, with our new TAME algorithm we are able to probe the layer with unprecedented accuracy [D.G. Dommermuth and R.C.Y. Mui, "The Initial Stages of a Microbreaking Wave," in *Proceedings of the 20th Symposium on Naval Hydrodynamics* , Santa Barbara (1994), to appear].

Significance: The TAME algorithm has applications to all surface and volume discretization methods. This algorithm is a unique approach for parallel computers and offers significant improvements in accuracy, flexibility, and efficiency relative to more conventional numerical techniques. By implementing the TAME algorithm, we expect to gain an improved understanding of how the atmosphere transfers energy and momentum to the ocean surface, which may lead to a better model of global warming.



Contour plot of the vortical structure of a near-breaking gravity-capillary wave

Development of a Coupled CFD/CSD Methodology

Joseph D. Baum and Hong Luo
SAIC, McLean, VA
Rainald Löhner
George Mason University, Fairfax, VA
Defense Nuclear Agency

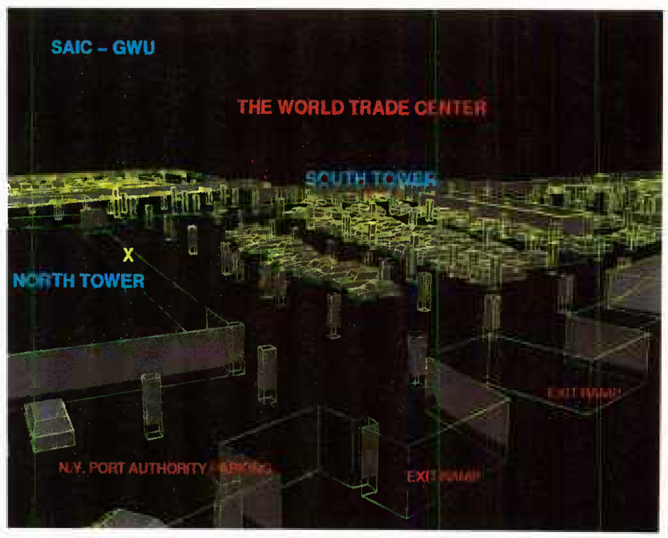
Computer Resource: Cray C-90 [NASA-Ames, Moffett Field, CA] and Cray M-98 [DNA, LANL, NM]

Research Objective: To develop a novel, fully integrated computational fluid dynamics (CFD) and computational structural dynamics (CSD) methodology for transient simulations and to enable the simultaneous determination of the free-field propagation of blast waves initiated by either conventional or nuclear weapons, the loads exerted on the structures by the impinging shocks, the structural deformation and kinematic motion, and the resulting modifications to the flowfield.

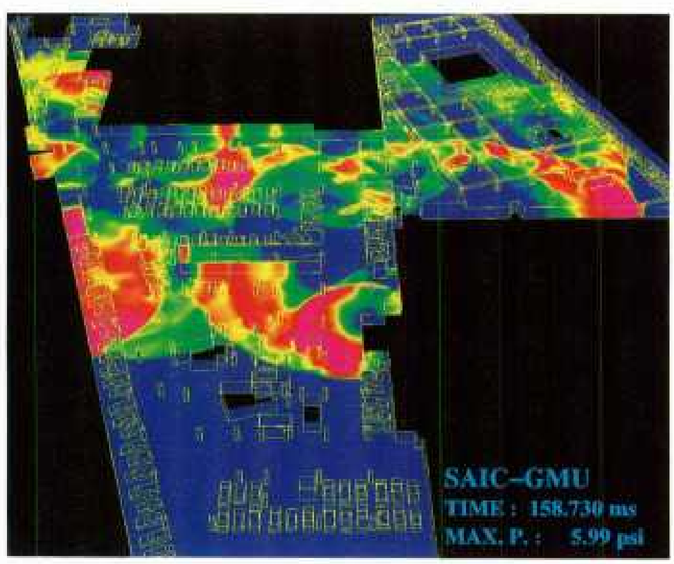
Methodology: Fully integrated state-of-the-art CFD and CSD algorithms were used. The CFD methodology, FEFLO96, is a recently developed, three-dimensional, adaptive, finite-element, edge-based, ALE shock-capturing methodology on unstructured tetrahedral grids for solving the Euler and Reynolds-averaged turbulent, Navier-Stokes equations. FEM-FCT was the high-resolution monotonicity-preserving algorithm used. The CSD methodology, DYNA3D, employed unstructured grids, a spatial discretization using finite-element techniques, large deformation formulation for the solids, explicit time integration, and several material models, kinematic options, and equations of state.

Results: This method has been applied successfully to both military applications, such as blasts in underground shelters where pre-test predictions were in very good agreement with available experimental data, and to civilian applications, such as the study of the blast in the World Trade Center.

Significance: This coupled methodology enables the understanding and improved prediction of both the shock waves diffraction phenomena and the structural response to blast loading.



Geometry definition of the B-2 garage level, World Trade Center



Pressure contours after 159 ms

Turbulent Mixing in Explosions

A.L. Kuhl and J.B. Bell
Lawrence Livermore National Laboratory, Livermore, CA
R.E. Ferguson and J.P. Collins
Naval Surface Warfare Center, Silver Spring, MD
Defense Nuclear Agency

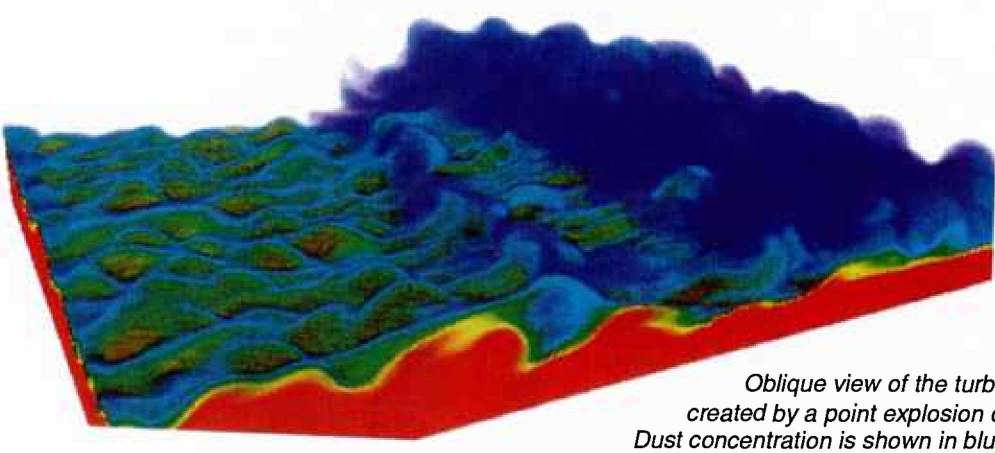
Computer Resource: Cray Y-MP [LANL, NM]

Research Objective: To develop general CFD tools for accurate predictions of the turbulent fields in explosions without resorting to turbulence models (which require an extensive and expensive database to tune the modeling parameters).

Methodology: Convective mixing simulations of turbulent fields were performed, based on high-order Gudonov solutions of the three-dimensional conservation laws. Adaptive mesh refinement (AMR) was used to capture enough of the turbulence spectrum to reach the inertial range. Subgrid modeling of molecular processes was used. The 3-D solution was averaged to extract mean and rms fields for engineering analyses. The convective mixing approximation was checked by performing 3-D Navier-Stokes calculations for limited spatial domains. The numerical model was verified by comparison with well-controlled laboratory experiments.

Results: This methodology was applied to the numerical simulation of the turbulent dusty boundary layer flow induced by a point explosion above a ground surface [A. L. Kuhl, et al. (1994) "Evolution of Turbulent Fields in Explosions," *Japanese National Shock Wave Symposium*, edited by K. Takayama, Tohoku University Press, Sendai, Japan]. Principal results include the evolution of the turbulent velocity field near the surface. Mean velocity profiles evolved with time. Initially they agreed with measurements of a dusty boundary layer behind a shock; at intermediate times they resembled the dusty boundary layer profiles measured in a wind tunnel; while at late times, they approached a 1/7 power-law profile. Velocity-fluctuation profiles were qualitatively similar to those measured for a turbulent boundary layer on a flat plate. The power spectrum has a slope of -5/3 in the inertial range.

Significance: This approach can be used to predict the evolution of other turbulent fields in explosions such as turbulent mixing at unstable interfaces, turbulent combustion, and turbulent transport of clouds and plumes. Such environments have important military significance for both offensive and defensive purposes such as drag loads on structures, afterburning in explosions, turbulent combustion in guns, fuel-air explosions, and hazards from chemical and biological clouds. These CFD codes can also be used for "dual-use" applications, e.g., to predict the evolution of turbulence combustion fields in engines.



Oblique view of the turbulent boundary layer created by a point explosion over a dusty surface. Dust concentration is shown in blue. Dust accumulates in the wall jet (on right) and in Goertler vortices (on left).

Reactive Flow Simulations with Detailed Chemistry

James W. Weber, Jr.
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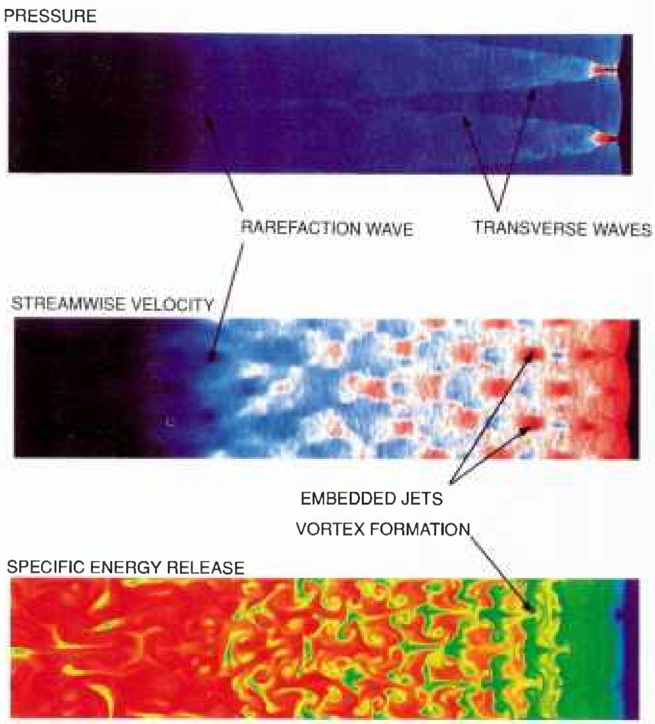
Elaine S. Oran
Naval Research Laboratory, Washington, DC
John D. Anderson, Jr.
University of Maryland, College Park, MD
Air Force Office of Scientific Research, Washington, DC

Computer Resource: TMC CM-5 [NRL, Washington, DC; AHPCRC, Minneapolis, MN]

Research Objective: To demonstrate the ability of the massively parallel CM-5 to produce computations of detailed reacting high-speed flows of importance to high-speed propulsion systems. To compute the chemical structure of a propagating detonation with a full, detailed chemical reaction mechanism, which can be used as a basis for evaluating the use of simplified chemical models.

Methodology: A two-dimensional, time-dependent, chemically reacting Navier-Stokes code was developed and optimized for the Connection Machine. The convection algorithm is a fully parallelized version of the NRL's Laboratory for Computational Physics' flux-corrected transport implementation of the FCT algorithm. A new method implemented for load balancing of the chemistry integration has enabled us to integrate the chemical equations representing the full, detailed chemical reaction process for hydrogen-oxygen (50 reaction rates, 9 species) at a cost less than the cost of integrating the convection.

Results: On standard scalar or vector supercomputers, the chemistry integration is the most costly part of the computation. With the new parallel implementation, the time for a computation can now be reduced by factors of 5 to 10. This technique has been applied to the computation of a detonation propagating in a tube, as shown in the accompanying figure. A detonation propagating in a low-pressure mixture of hydrogen and oxygen heavily diluted with argon is known to produce relatively uniform transverse wave patterns as it propagates. The computed flowfield shows the structure in a 2048 by 256 computation.



Propagating detonation in a low-pressure system of hydrogen-oxygen gas heavily diluted with argon. Images at 416 μs (step 24000) on 2048 x 256 grid.

Significance: Computing the detailed chemical structure of a flow at less than twice the cost of computing the behavior of an unreacting flow opens up the possibility of using more accurate chemical models for describing propulsion systems and engines. For example, this approach greatly changes what we can do to design or optimize propulsion systems or evaluate the minor species that are the pollutants in propulsion and waste disposal systems. In terms of the basic reactive-flow physics, we can now look with new accuracy at the effects of chemical reactions on turbulent flows.

Reflected-Shock/Boundary-Layer Interaction in Shock Tubes

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E. S. Oran and J.P. Boris
Naval Research Laboratory, Washington, DC
J. D. Anderson, Jr.
University of Maryland, College Park, MD
Air Force Office of Scientific Research, Washington, DC

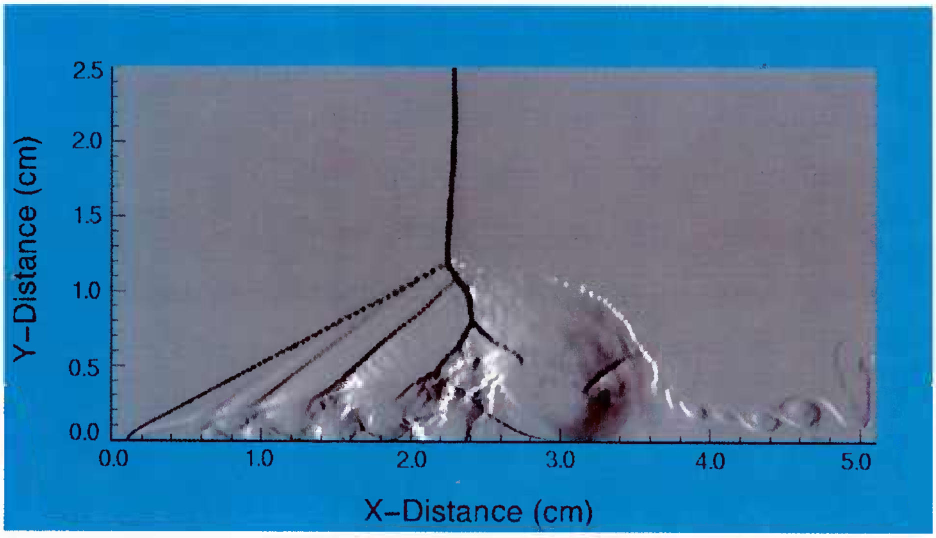
Computer Resource: TMC CM-5 [NRL, Washington DC; AHPCRC, Minneapolis, MN] and TMC CM-200 [NRL, Washington, DC]

Research Objective: To study the two-dimensional, unsteady, viscous interaction aspects of shock bifurcation in the reflected region of shock tubes. The impact of heat transfer, Reynolds number, incident shock strength, and finite-rate chemical dissociation on the interaction was also investigated.

Methodology: The numerical simulation implements a data-parallel version of the flux-corrected transport (FCT) algorithm, which includes the viscous terms of the Navier-Stokes equations. The program is written in data parallel using CMFortran. Special effort has been made to incorporate the boundary conditions and the inflow model directly into the calculation, resulting in a computationally efficient algorithm.

Results: Under certain conditions, the reflected-shock/boundary-layer interaction results in the formation of unstable shear layers with attendant large displacements of the core flow. Increasing shock strength and chemical dissociation enhance interaction size. Wall cooling leads to a diminished interaction [Y.S. Weber, J.D. Anderson, Jr., E.S. Oran, and J.P. Boris, "The Numerical Simulation of Shock Bifurcation near the End Wall in a Shock Tube," AIAA Paper 94-2307, 25th AIAA Fluid Dynamics Conference, Colorado Springs, CO, June 1994].

Significance: These studies are motivated by the requirement to model the high-enthalpy flow conditions associated with high-speed flight and missile aerodynamics. Understanding this flow has important implications for interpreting experimental data and designing more effective advanced vehicles and testing techniques.



Structure of the bifurcation region for an $M_s = 10$ shock/boundary-layer interaction in air. Density gradient contours are shown.

Three-dimensional Radiation Transport Hydrodynamics

David E. Fyfe, Jill P. Dahlburg, and John H. Gardner
Naval Research Laboratory, Washington, DC

Computer Resource: TMC CM-5 [NRL, Washington, DC]

Research Objective: Radiation transport hydrodynamics codes have many applications in high-temperature physics, including the study of laser matter interaction (LMI). Applications range from the design of high-gain inertial confinement fusion (ICF) pellets to the design and diagnosis of near-term laboratory experiments for the NRL NIKE KrF Laser Facility. Realistic LMI simulations of the ablative Rayleigh-Taylor (RT) instability offer one of the best means of learning how to control this instability, which is the most dangerous hydrodynamic instability to affect laser ablatively accelerated targets.

Methodology: RAD3D_CM is a compressible hydrodynamics code that contains the following effects relevant for simulating high-temperature plasmas: inverse bremmstrahlung laser energy absorption, classical Spitzer thermal conduction, real (table look-up) equations-of-state with either separate or identical electron and ion temperatures, and multigroup variable Eddington radiation transport. On the CM-5, RAD3D_CM exhibits more than a seventy-fold increase in speed over its serial XMP-running predecessor, RAD3D. Combined with the large CM-5 memory, this enables us to simulate a wide range of three-dimensional multimode problems that have hitherto been impossible. [D.E. Fyfe, J.P. Dahlburg, and J.H. Gardner, 23rd Anomalous Absorption Conference, June 1993.]

Results: We are currently using RAD3D_CM to simulate the evolution of 85-μm-thick NIKE simple plastic (CH) ablator targets accelerated with prototype ICF driver conditions. Our well-resolved simulation results indicate that ablative RT perturbations on optimized laser targets do not grow turbulent during timescales of interest. We find that the subset of RT unstable modes most dangerous to target survival are those that evolve to more spherical bubbles, are of the highest wavenumber not subject to strong density gradient stabilization, and are present from very early times. The dominance at late times of the initially seeded spherical bubbles can be seen in the figure; the laser-direction (x) integrated mass density has been plotted as a function of the spatial directions transverse to the incident laser (y,z) at times $t = 0$ ns, $t = 2.5$ ns, and $t = 4.7$ ns.

Significance: The code RAD3D_CM is the first three-dimensional LMI radiation transport hydrodynamics code to include all relevant physical effects. The calculations performed with RAD3D and with RAD3D_CM, which are the first to show that the effect of RT perturbation shape is robust and large enough to be experimentally detected, are assisting us to design targets for upcoming NRL NIKE Laser Facility experiments. Beyond the need for improved combustor and furnace design, this capability, together with related simulation and laboratory experiments, will enable us to replace underground nuclear weapons testing with a comprehensive laboratory-scale, nuclear-weapons and weapons-effects simulation program with no environmental impact, at greatly reduced yearly outlay.

Integrated mass density: initially (left); after 2.5 ns (center); after 4.7 ns (right)

Time-Varying Flames

Carolyn R. Kaplan
Naval Research Laboratory, Washington, DC

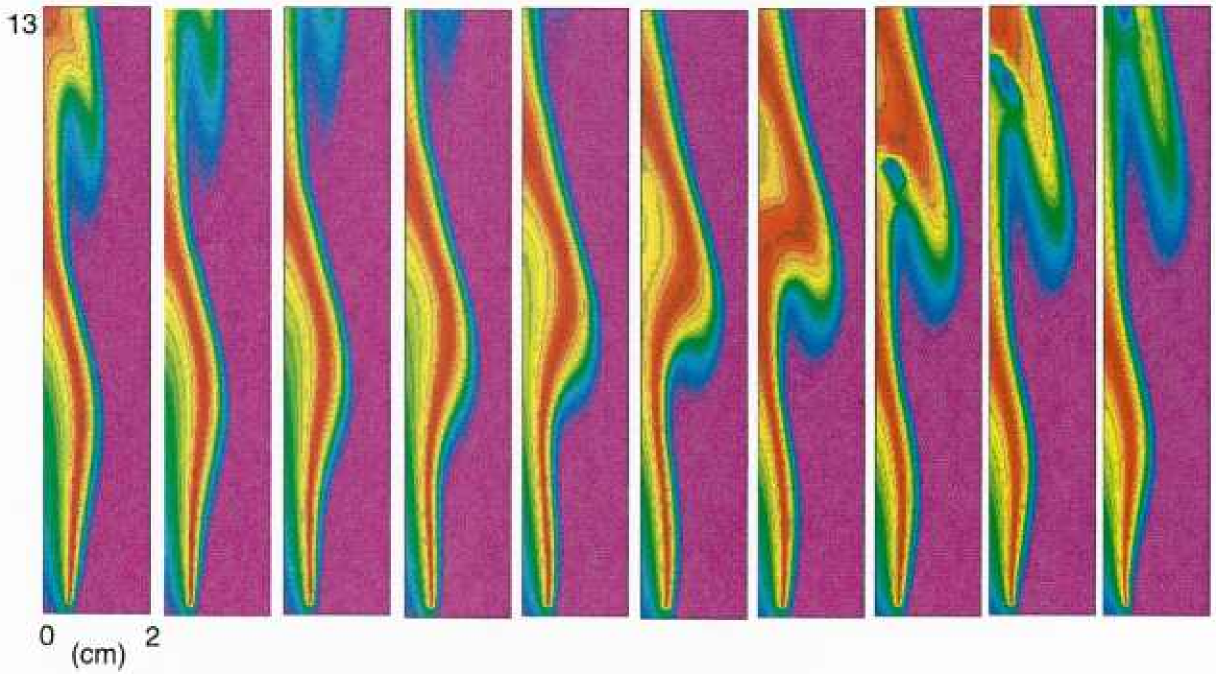
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: Experimental measurements of a coflowing acoustically forced flickering methane/air flame at the National Institute of Standards and Technology show that soot production is four times greater than that measured for a steady flame with the same mean fuel flow velocity. Simulations are conducted to better understand the causes for the enhanced soot production in the time-varying flame.

Methodology: The numerical model solved the time-dependent, multi-dimensional, reactive-flow Navier-Stokes equations coupled with submodels for soot formation and radiation transport. Fluid convection was solved with a high-order implicit algorithm, barely implicit correction to flux-corrected transport, while thermal conduction, molecular diffusion, and viscosity were evaluated with explicit two-dimensional finite differencing. Species conversion/energy release and soot formation processes were modeled phenomenologically. Each simulation required approximately 4 hours on the Cray C-90.

Results: The shapes of the simulated and experimental flames are similar, and both exhibit tip clipping (flickering portion clips off at the top). Like the experiments, the computations also show that the soot volume fraction in the clipped portion of the flickering flame is approximately three to four times greater than that computed for the steady flame. The simulations showed that differences in residence times, temperatures, and local stoichiometric conditions between the steady and time-varying flames cause dramatic increase in soot production. That is, in time-varying flames, soot production occurs over significantly longer residence times during which the temperatures and local stoichiometries are very favorable for soot growth.

Significance: Details obtained from simulations such as these are used to build models of DoD vehicle fire safety.



Flickering methane-air diffusion flame. Sequence of temperature contours in time shows clipped off portion of the flame. Interval between frames is 10 ms.

Two-dimensional Version of Sabot Discard

B. Kevin Edgar, Steven Anderson, and Paul Woodward
Army High Performance Computing Research Center, Minneapolis, MN
Army Research Office, RTP, NC
Kurt Fickie
Army Research Laboratory, Aberdeen Proving Ground, Aberdeen, MD

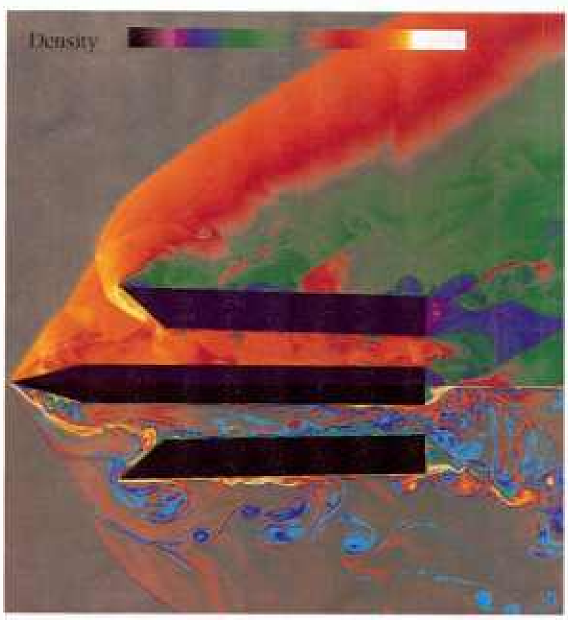
Computer Resource: TMC CM-5 [AHPCRC, Minneapolis, MN]

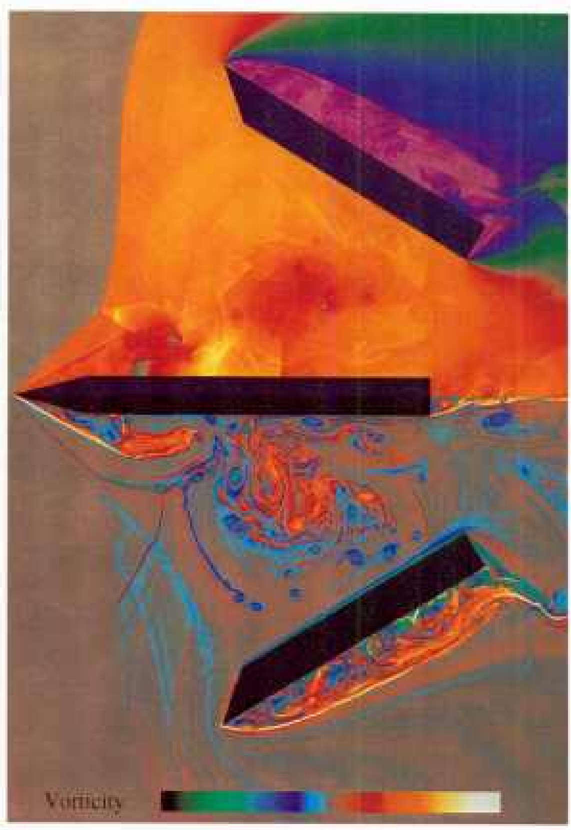
Research Objective: To develop and test a version of the two-dimensional PPM code for simulating transient supersonic flows about objects that move under the influence of the pressure forces exerted by the surrounding flow.

Methodology: The PPM code was modified to treat moving rigid obstacle boundaries using a variation of multi-fluid interface tracking techniques and to move the obstacles according to the pressure forces exerted by the flow. The new code was implemented on the CM-5, and this test problem, inspired by the sabot discard process, was run at grid resolutions of the 1280 x 1024 and of 2560 x 2048 zones.

Results: Performance was achieved with 8 Gflops, and the motion of the 2-D "sabot" was nearly the same on both computational grids. The new, experimental method of treating the obstacle boundaries and motion, which is especially easy to parallelize, gave the best results for the finer grid. Further tests will be made, but these initial results are quite promising.

Significance: Developing techniques to simulate the sabot discard process efficiently and easily on massively parallel computers will help to shorten the present 10-year design cycle for these important weapons. The same computational techniques should apply to simulating the interaction of fluids and rigid structures in other contexts such as high-speed flight.





Simulation of a 2-D version of projectile sabot discard; left: density contours at 0.253 ms; right: vorticity at 1.49 ms

Design of Compact Exhaust Nozzles for Turbine Missile Engines

M. K. Lockwood and W. Z. Strang
Wright Laboratory, Wright-Patterson Air Force Base, OH

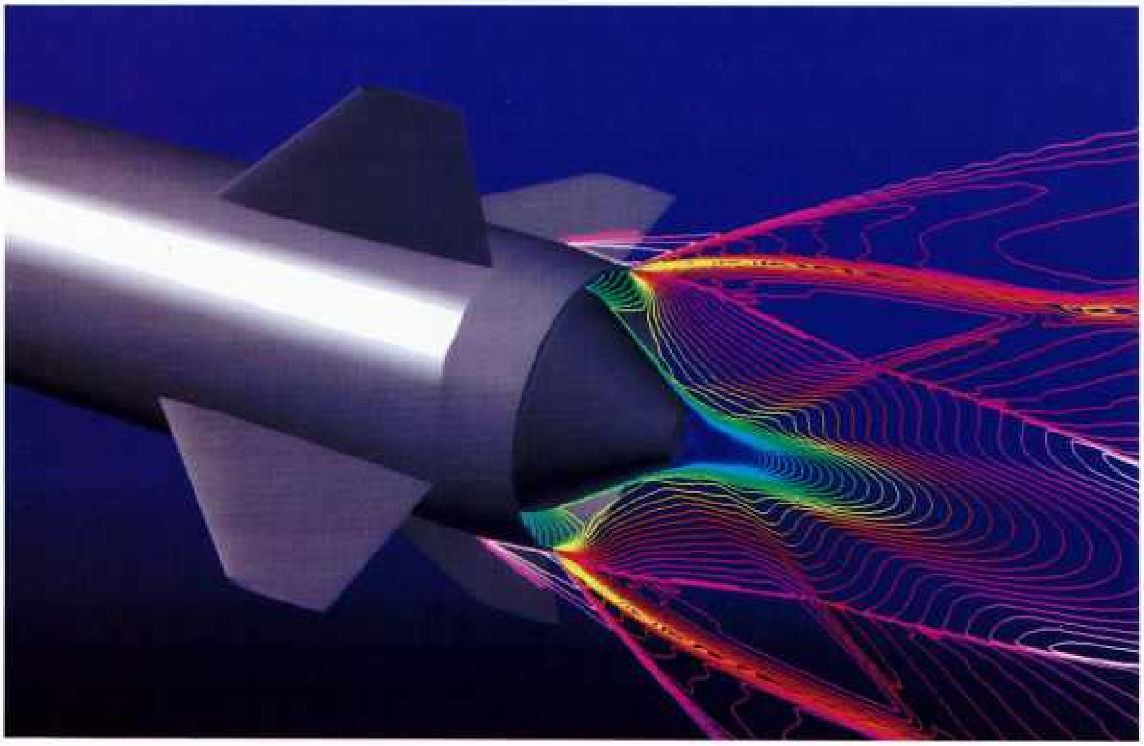
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To minimize nozzle cost and maximize range of theater defense missiles. Nozzle cost is minimized by choosing a single position nozzle. Since overall missile length is fixed by current launcher designs, maximizing missile range results is a tradeoff between nozzle length and fuel capacity. The optimum nozzle possesses the appropriate combination of reduced length and high performance to maximize vehicle range.

Methodology: The design of the nozzle to optimize thrust minus drag coefficient was based on the Taguchi design of experiments method. Four design variables were chosen—cowl length, cowl angle, plug angle, and nozzle length. Two CFD codes were used to provide the thrust minus drag coefficient for the eight nozzles defining the Taguchi matrix. One of the codes, Cobalt, is an unstructured grid code developed at Wright Laboratory. The ideas of Godunov, Collela, and van Leer form the foundation for the inviscid algorithm while the construction of the viscous terms follows MacCormack's work. The Baldwin and Barth turbulence model simulates the effects of fine-scale turbulence.

Results: The combined Taguchi and CFD methodology was successful in optimizing the nozzle within the design space considered and produced a nozzle with performance greater than that of the baseline nozzle. The improvement is 5.3% and 3.7% at Mach 3.5 and Mach .5, respectively.

Significance: An optimum nozzle has been designed for the missile-sized expendable turbine engine. The use of CFD increased the design space investigated and reduced the design cost as compared to a purely experimental development.



Mach contours on optimum nozzle at Mach 3.5, NPR = 63.04

Large and Small Submarine Appendage Computational Fluid Dynamic Analysis

Troy A. Hollingsworth
Naval Undersea Warfare Center, New London, CT

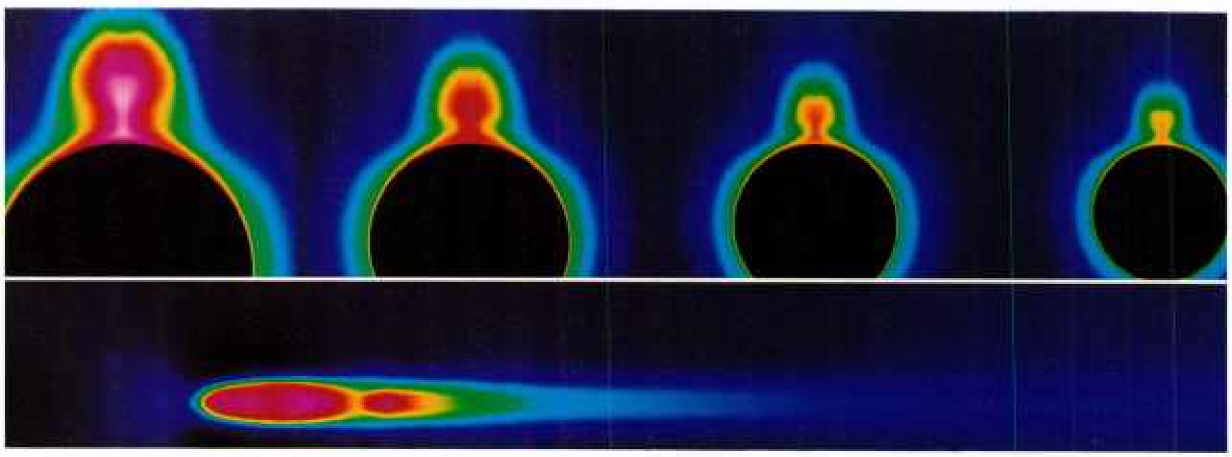
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To investigate hydrodynamic effects of appendages on the submarine flowfield for varying submarine speeds. Both large (on the order of a submarine sail) and small appendages were studied.

Methodology: A finite-difference Reynolds-averaged Navier-Stokes solver was used in a curvilinear coordinate system. The goal was to capture vortices and recirculation zones as well as pressure profiles on the submarine itself. Both algebraic and two-equation turbulence models were used. A fully multi-tasked (95% to 97% parallel) and vectorized alternating direction implicit (ADI) solver was used, and eight processors were simultaneously tasked. A multi-layered approach was implemented to provide faster turnaround. Mesh sizes across the layers ranged from 10,000 to 3,000,000 nodes. The large meshes generally required 32 to 96M words of main memory. The multi-layered approach significantly reduced total run time by efficiently providing a near-solution first guess to the final mesh. It also allowed the debugging process to be completed on the smallest meshes. Because of the multi-layered approach, run times that had required 150 CPU hours in the past were completed in under 30 CPU hours.

Results: The results provide insight to the ramifications of a given design on submarine flowfields. Important information includes potential noise sources resulting from recirculation zones and nonuniform flow at the propulsor inlet.

Significance: Hydrodynamic effects of appendages are important to the performance and detectability of a submarine. Appendages potentially affect submarine maneuverability, hydrodynamic performance, and signatures. Computational analysis can provide a cost-effective tool for appendage design, leading to higher performance without higher detectability and thus, broader mission capability.



Vertical-cut planes (top row) and horizontal-cut plane (bottom row) of streamwise velocity aft and over the appendage (blue is free stream; magenta is reverse flow)

Predicting Parachute Performance

Richard J. Benney and Keith R. Stein
U.S. Army Natick Research Development & Engineering Center, Natick, MA

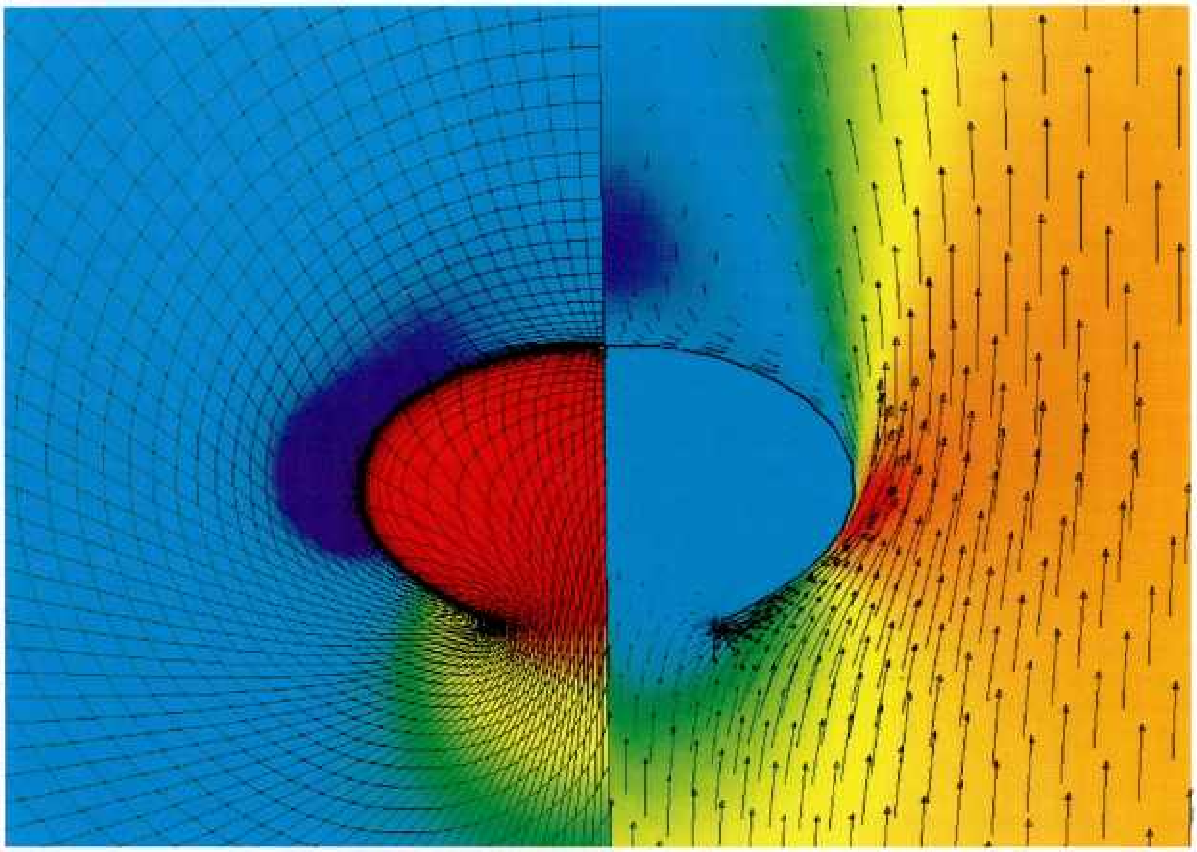
Computer Resource: Cray-2 [TACOM, Warren, MI]; Kendall Square Research KSR1-256 [ARL, Aberdeen Proving Ground, MD]; and Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To numerically predict parachute openings and terminal descent characteristics and to develop a computational parachute design tool to reduce the cost of development and testing.

Methodology: This research involves modeling the fluid-structure interaction problem between the parachute system and the surrounding flowfield by numerically coupling a computational fluid dynamics (CFD) code to a structural dynamics code.

Results: The simulations performed for openings of round parachutes compared favorably with experimental data. The current computational model's development time was greatly reduced by the availability of Cray supercomputers at ARL, CEWES, and TACOM. The figure illustrates the calculated flowfield around a fully opened, reefed G-12 round parachute. Further development in this effort will depend on the availability of high performance computers.

Significance: This effort provides a computational design tool that will enhance the current "cut and try" design process. This will significantly decrease costs associated with design and testing while enhancing our understanding of parachutes for both military and civilian benefit.



Reefed G-12 flowfield; (left) pressure field, (right) velocity field

Wall Pressure Fluctuations Beneath a Turbulent Boundary Layer

Peter A. Chang III
Naval Surface Warfare Center, Bethesda, MD

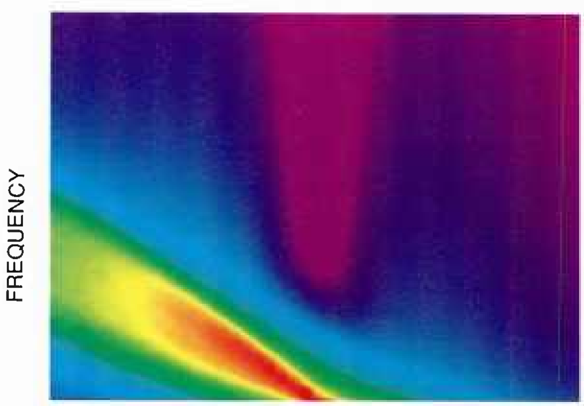
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: To use turbulence simulations to learn the physics of wall pressure fluctuations (WPFs), which generate flow-induced noise in flows over aircraft fuselages, acoustic arrays, and sonar domes. Unlike Reynolds averaged Navier-Stokes (RANS) solvers, turbulence simulations provide time-accurate turbulent flow data.

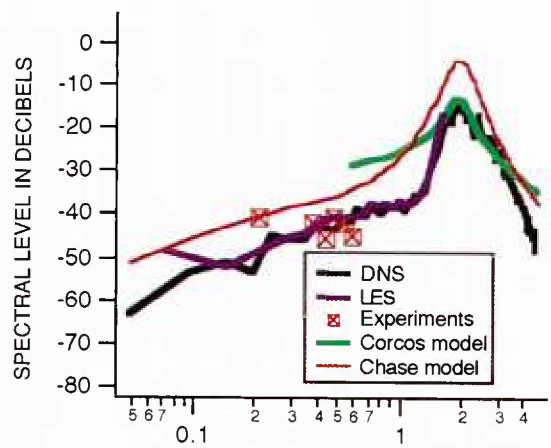
Methodology: The developed flow solver integrates the incompressible Navier-Stokes equations in a channel flow that is periodic in the streamwise and spanwise directions. Starting from a laminar channel flow, the flow is perturbed and develops into a fully developed turbulent flow. This is further integrated in time until sufficient time series data are obtained to compute wavenumber-frequency spectra. Simulations can be either direct numerical simulations (DNS), where all significant energy-containing scales are resolved, or large eddy simulations (LES), where only the largest scales are resolved, with the energy balance maintained with a subgrid scale model. For this study, a DNS was run that had 1.8M grid points, requiring 32M words of core memory and 350 CPU hours on the Cray C-90. LES require significantly less resources; a grid of 0.4M points required 12M words of memory and 60 CPU hours on the Cray Y-MP.

Results: A LES wavenumber-frequency spectra plot and a constant frequency cut that compares spectra from the simulations with experimental data and semi-empirical models are shown below. The wavenumber-frequency spectra of the wall pressure from simulations compare very well with experimental data. The slope of the spectra in the region is quadratic in wavenumber, which had been predicted analytically.

Significance: The simulations have provided databases with which to study WPFs in wavenumber-frequency and space-time domains. We are presently using the data to study the relationship between velocity fields and wall pressure. This may lead to improvement of semi-empirical models that predict WPFs. Comparison of the LES and DNS spectra shows that we may be able to use the relatively cheaper (computationally) LES for simulations involving active and passive control of WPFs.



2-D streamwise wavenumber-frequency plot of wall pressure spectra from LES



Comparison of simulations, experiments, semi-empirical models; constant frequency cuts and semi-empirical models

Viscous Free-Surface Flow Around Ships

H.J. Haussling and R.W. Miller
Naval Surface Warfare Center, Bethesda, MD

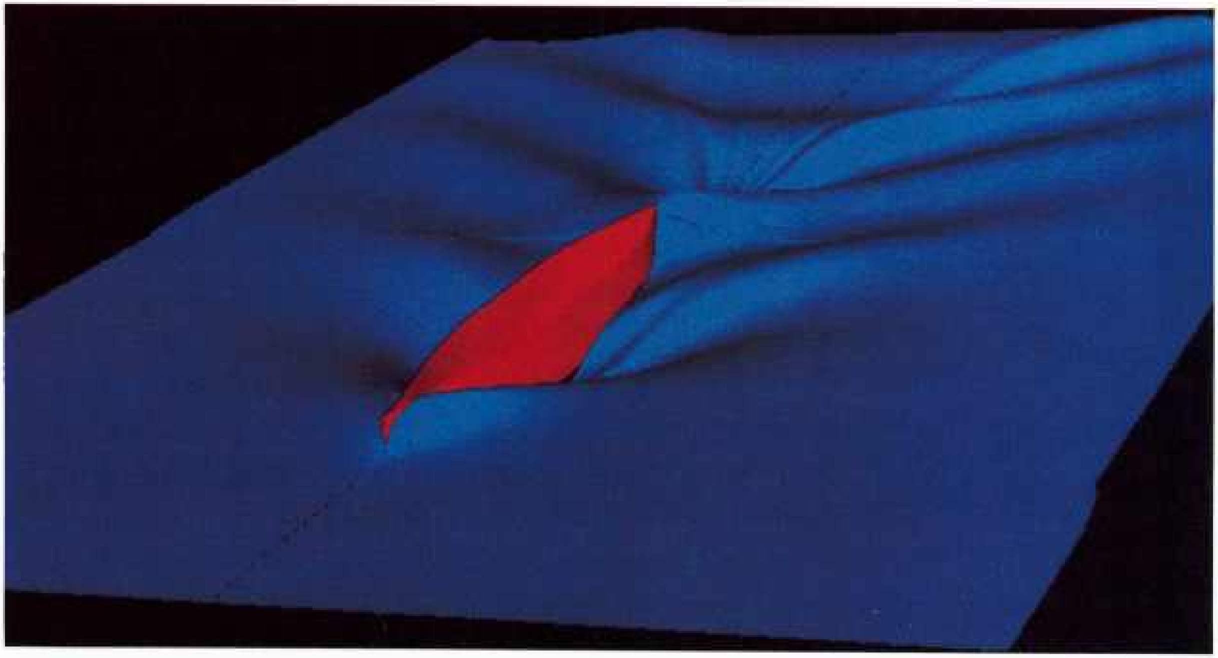
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: Considerable progress has been made in recent years on the use of computers to study naval fluid dynamics. In particular, useful computer codes have been developed for solving the equations for flow around surface ships with neglect of frictional (viscous) effects. Simultaneously, progress has been made on solving the equations for flow with viscous effects but away from the water surface. The objective of this work is to combine these two areas of progress (viscous and water surface) for the study of naval vehicles operating in or near the air/sea interface.

Methodology: Methods and computer software were previously developed and validated for the computation of flows around submerged bodies, with and without appendages. The computational treatment of free-surface boundary conditions has now been included in this capability. The approach was to start with linearized conditions and work toward the use of fully nonlinear and fully viscous free-surface conditions. The tremendous number of data points that must be computed to represent the pertinent physics requires the use of the largest and fastest available scientific computers.

Results: Viscous free-surface flow was computed around a typical hull shape for which measured data were available (see figure). These results have been presented and compare very favorably with experimental results and with other computed solutions presented [H.J. Haussling and R.W. Miller, "Reynolds-averaged Navier-Stokes Computation of Free-surface Flow about a Series 60 Hull," presented at CFD Workshop Tokyo, Ship Research Institute, Tokyo, Japan, March 23, 1994].

Significance: This work provides a powerful tool that couples free-surface boundary conditions with a solution of the equations for flow around fully or partially submerged bodies. With such coupling, viscous flow around submarines near the water surface and around surface ships can be computed, and the influence of the water surface on such flows can be examined. Such computations include the generation of vortices in the flow around the bodies and the resulting interaction of the vortices with the free surface, including their influence on the surface wave pattern.



Computed waves in the flow around a surface ship model

Structure of Vortex Breakdown Above a Pitching Delta Wing

Miguel Visbal
Wright Laboratory, Wright-Patterson Air Force Base, OH

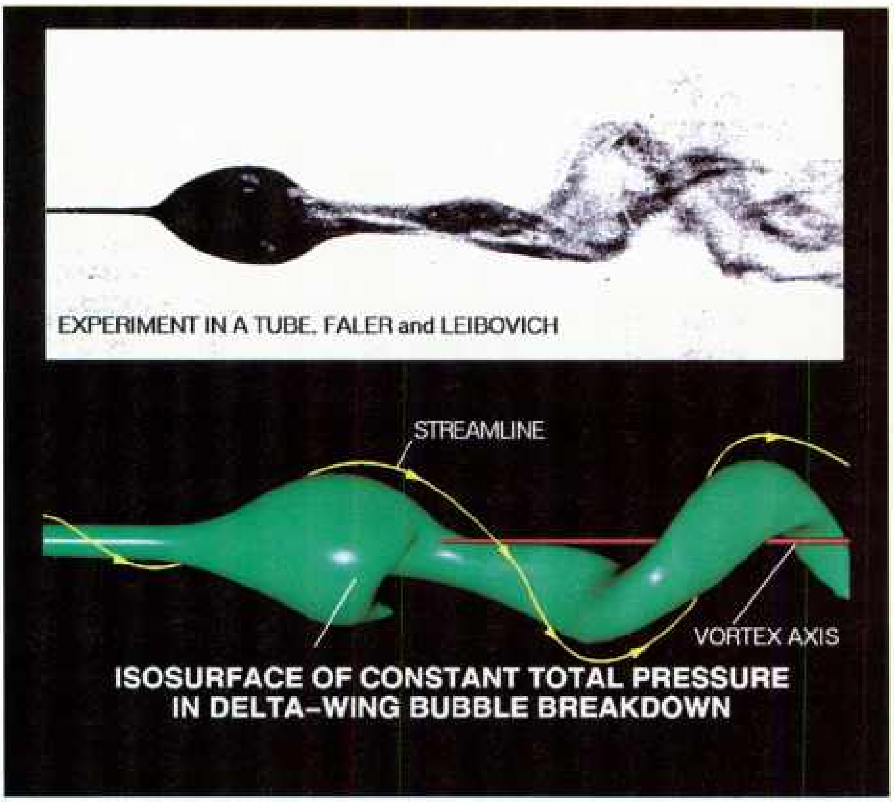
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To study the onset, transient behavior and three-dimensional flow structure of vortex breakdown above a slender delta wing maneuvering to high angle of attack.

Methodology: The flows were simulated by solving the full unsteady 3-D Navier-Stokes equations on a moving grid using the implicit beam-warming algorithm. The flow solver has been fully validated and optimized for a vector machine.

Results: Results were obtained for a delta wing pitching at constant rate to a high incidence. Excellent agreement with experimental measurements was achieved in terms of breakdown location and velocity. The 3-D flow structure was described for the first time in the framework of critical-point theory ["Onset of Vortex Breakdown Above a Pitching Delta Wing," *AIAA J.*, **32** (Aug. 1994)].

Significance: The capability to accurately simulate the phenomenon of vortex breakdown above a wing is a key issue for the prediction of aircraft dynamics and control at high angle of attack. This capability provides a cost-effective means of investigating methods for vortex breakdown control to reduce tail buffet and structural fatigue in maneuvering air vehicles.



Comparison of computed and experimental vortex breakdown bubble

Dynamics of Noncircular Jets

F. F. Grinstein and Upul Obeysekare
Naval Research Laboratory, Washington, DC

Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To better understand the basic mechanisms for active and passive control of jet dynamics. This knowledge is needed to increase the range and speed of airbreathing and rocket propulsion systems. The issues addressed aim at attaining more efficient and environmentally cleaner combustion engines.

Methodology: Three-dimensional computer simulations of the low-aspect-ratio (AR = 1-4) rectangular jets of practical interest in the subsonic applications were performed. The underlying fluid-mechanical processes that control jet development and lead to the transition to turbulence were characterized as well as the effects these processes have on entrainment, mixing, and combustion. The 3-D reactive-jet numerical model used involves a monotonically integrated large-eddy simulation approach, appropriate inflow/outflow open boundary conditions, and multi-species diffusive transport and finite-rate chemistry. The well-resolved 3-D simulations required for this project demand large amounts of computer memory and time, which are available only at facilities such as those provided by the DoD HPCMP at CEWES.

Results: The simulations showed that the basic jet development is controlled by the dynamics of formation, merging, and breakdown of vortex rings and hairpin vortices. They provided an insight into the underlying fluid dynamical processes involved in the transition to turbulence. The studies demonstrated the entrainment-enhancing flow dynamics leading to the experimentally observed axis-switching phenomena in noncircular jets. This documented for the first time the detailed dynamics and topology of vortical structures in rectangular jet nozzles, including the effects of density differences and exothermicity on the jet dynamics [F.F. Grinstein, "Vorticity Dynamics in Spatially-Developing Rectangular Jets," AIAA paper 93-3286, AIAA, Washington, DC, 1993].

Significance: Noncircular jets are of considerable interest because of their larger entrainment rates relative to those of comparable round jets. This feature is of great importance in practical applications demanding enhanced jet combustion and/or reduced plume signatures. It is also important in other fields where environmental requirements are for the jet nozzles to ensure rapid initial mixing and submergence of the effluent fluid.

Instantaneous visualization of a developed rectangular jet with aspect ratio 3:1 in terms of isosurfaces of the vorticity magnitude (gray) and positive/ negative streamwise vorticity (green/ gold), at 40% of the peak value. Flow is from bottom to top and is characterized by vortex rings that roll up from the initial rectangular vortex sheet and their strong interactions with superimposed (streamwise) braid vortices

Vortex-Ring/Free-Surface Interaction

Samuel Ohring and Hans J. Lugt
Naval Surface Warfare Center, Bethesda, MD

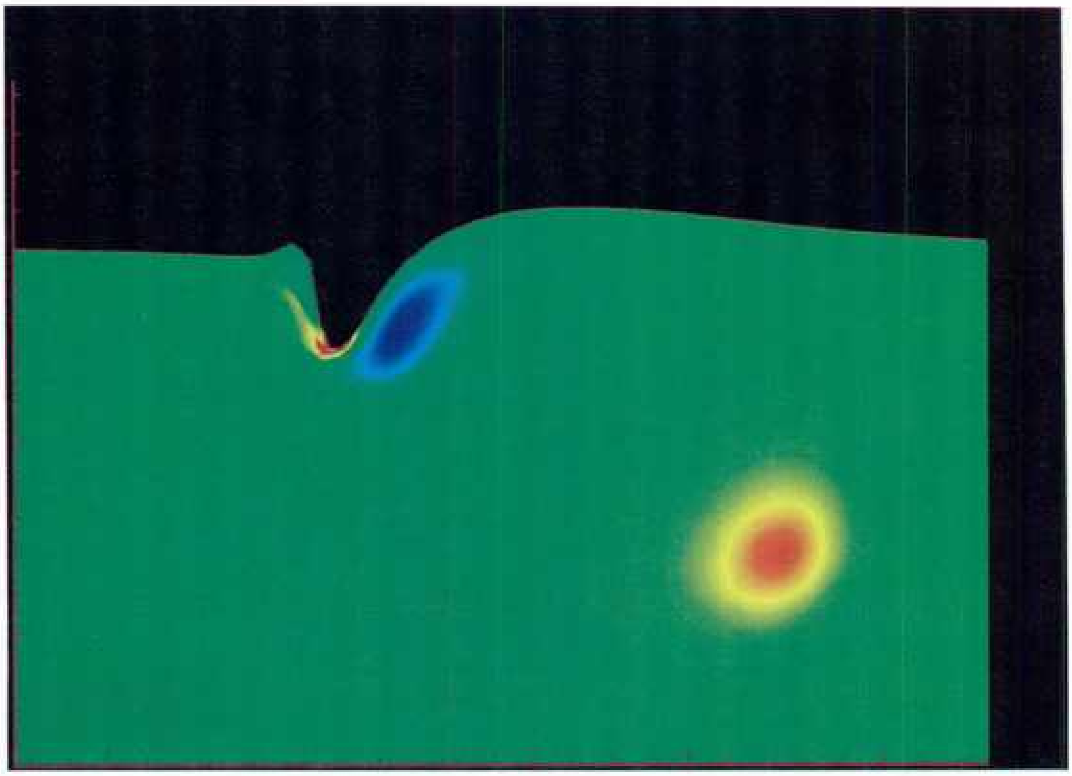
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To understand vortex-ring interaction with a free surface (the deformation and connection of a vortex ring during encounter with a free surface), which is subject to deformation. This understanding will help in the interpretation of surface signatures of wake flows.

Methodology: The three-dimensional Navier-Stokes equations for a viscous, incompressible fluid with full nonlinear free-surface conditions were solved with boundary-fitted coordinates, adaptive gridding, and artificial compressibility applied at each physical time step. This technique solves seven field equations for three velocity components, pressure, and three spatial coordinates. The number of grid points is more than three million.

Results: Numerical computations were made for a higher Reynolds number and a thinner vortex core than those previously chosen. The angle of inclination has been kept at 45°. No qualitative difference to the smaller Reynolds-number flow is observed. It is expected, however, that such qualitative differences will occur at other angles of inclination and at much higher Reynolds numbers. This is because the experimentally observed reconnection process at Reynolds number of the order of several thousand leads to a half ring, not to a cylindrical vorticity sheet as numerically computed. The average case took 96M words of central memory and 80 hours on the C-90.

Significance: The findings of this study contribute to the physical understanding of vortex/free-surface interaction, particularly the intricate reconnection process, and may help to obtain a complete picture of wave signatures behind ships and submarines.



Vorticity in the symmetry plane of the three-dimensional flowfield. Reynolds number: 200; Froude number: 0.1; 45° angle of inclination. Color spectrum of vorticity values: red (-203) to blue (116).

Oblique Shock-Wave/Vortex Interaction

D. P. Rizzetta
Wright Laboratory, Wright-Patterson Air Force Base, OH

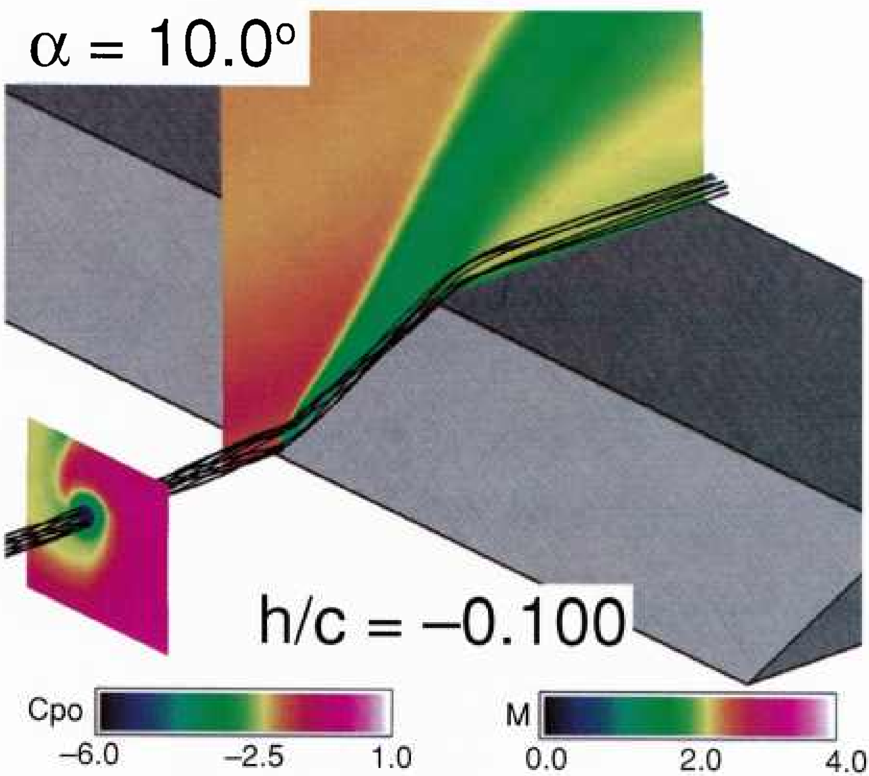
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: This work numerically simulates the interaction between a streamwise vortex and an oblique shock wave for high Reynolds number supersonic flows. The vortex develops at the tip of a vortex-generating fin, which is suspended from the ceiling of a wind tunnel. Downstream, an oblique shock wave is produced by a wing surface with a sharp leading edge.

Methodology: The governing equations were taken to be the compressible three-dimensional Euler and mass-averaged Navier-Stokes equations. Effects of turbulence were accounted for by a simple algebraic eddy viscosity model. Solutions to these equations were obtained via an implicit, approximately factored, finite-difference algorithm employing a fully vectorized, highly efficient computer code, which has been well validated.

Results: Numerical solutions have been generated for several values of the vortex generator angle of attack and corresponding vertical positions of the wing surface. Resultant features of the interactions have been elucidated, and comparison has been made with experimental data in terms of static pressure distributions on the wing surface. Most commonly observed physical details of the flowfield have been reproduced by the computations [D. P. Rizzetta, "Numerical Simulation of Oblique Shock-Wave/Vortex Interaction," AIAA Paper 94-2304, 25th AIAA Fluid Dynamics Conference, Colorado Springs, CO, June 1994].

Significance: Shock-wave/vortex interactions typically occur in supersonic fighter aircraft resulting in a loss of lift, an increase in drag, and a decrease in aerodynamic performance. Understanding the basic mechanisms of these interactions is the initial step in controlling them or eliminating their undesirable effects.



Total pressure contours of the vortex core(Cpo), Mach number contours above the wing surface (M), and particle paths where alpha is the vortex generator angle of attack and h/c the wing vertical height.

Parallel Implementation of Direct Simulation Monte Carlo

Choong Oh and Elaine S. Oran
Naval Research Laboratory, Washington, DC
Bohdan Cybyk
Wright Laboratory, Wright-Patterson Air Force Base, OH

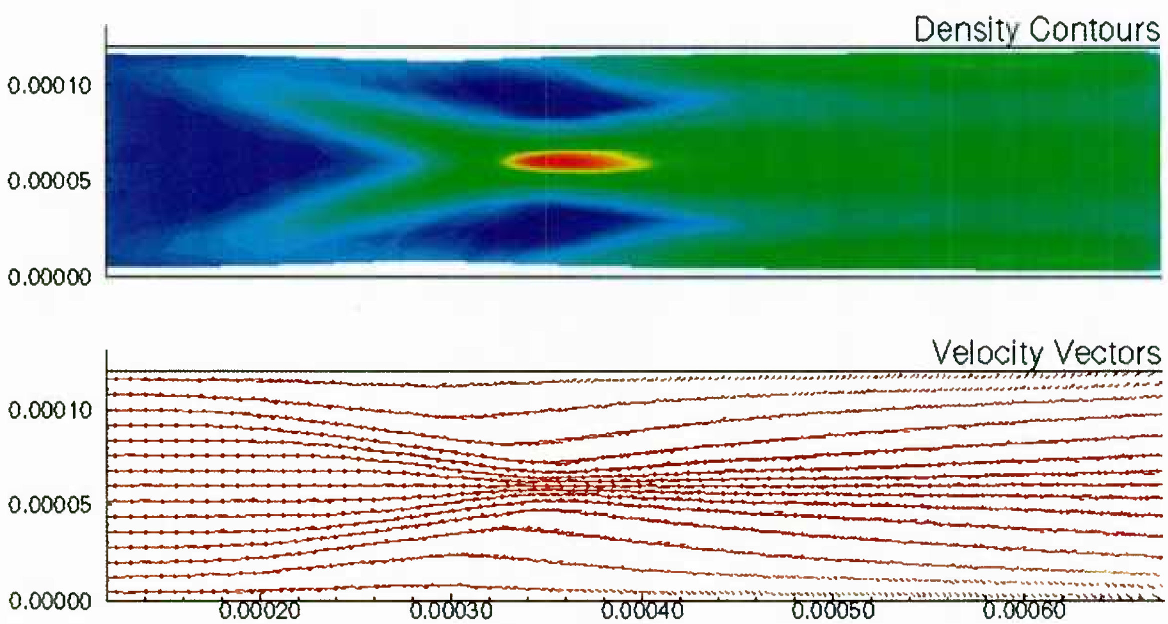
Computer Resource: TMC CM-5 [NRL, Washington, DC; AHPCRC, Minneapolis, MN]

Research Objective: To develop highly efficient, massively parallel techniques for simulating high-Knudsen-number flows by combining the Monotonic Lagrangian Grid (MLG) algorithm with the basic principles of the Direct Simulation Monte Carlo (DSMC) method. To use these algorithms to simulate hypersonic reentry flows and microflows.

Methodology: The DSMC, a statistically based particle method, was used to predict the behavior of a high-Knudsen-number channel flow. The MLG is a method of handling complex particle data structures. A main feature of this method is that the grid is dynamically defined by the particle locations, so that even as particles move, those particles that are near in physical space are near in computer memory. Both the DSMC and the MLG are optimum for the types of parallelization offered by the Connection Machine. Combining these two approaches provides a method that has automatic grid refinement according to number density, a necessary feature that is normally a very costly addition to standard methods.

Results: The DSMC and the MLG have been successfully combined, and the current effort involves parallelizing the DSMC and the MLG on the Connection Machine. When applied to a standard test problem, the parallel version is almost 200 times faster than the scalar workstation version.

Significance: The successful application of DSMC is based on the availability of high-speed computers with large memory. The DSMC model is required for computational re-entry hypersonic flight at intermediate altitudes for small projectiles and for microsystem design. We are testing this now by computing flows in microchannel systems with realistic materials and dimensions.



Mach 10 flow into a 1.2 µm channel containing helium gas. The computation shows the interactions of diffuse shocks and the formation of boundary layers.

Elementary Fluxtube Reconnection

Russell B. Dahlburg, Spiro K. Antiochos, David Norton, and Upul Obeysekare
Naval Research Laboratory, Washington, DC

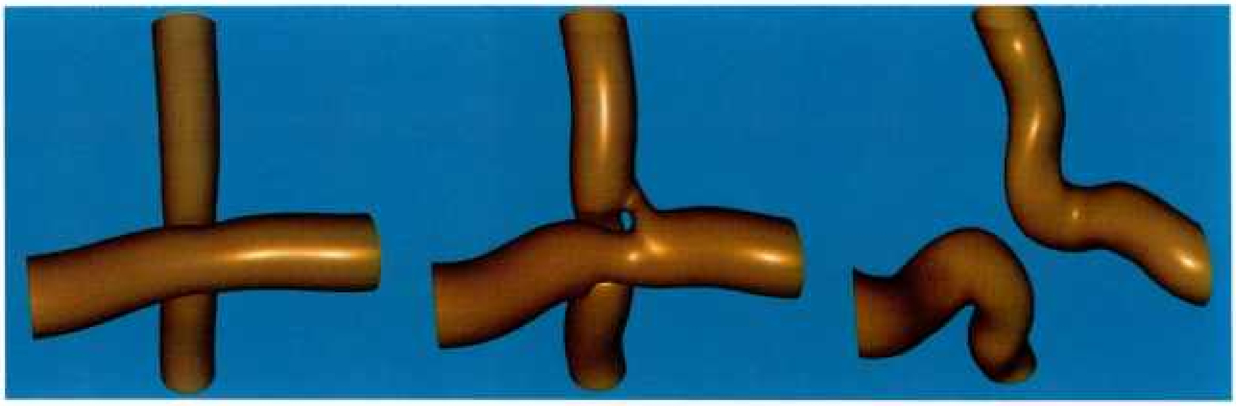
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS] and TMC CM-5 [NRL, Washington, DC]

Research Objective: To perform numerical simulations of colliding magnetic fluxtubes with the goal of explaining the observation of bursts in hard X-ray data from solar flares. The bursts are interpreted as resulting from the reconnection of pairs of magnetic fluxtubes.

Methodology: Numerical simulations were carried out using a three-dimensional generalization of our CRUNCH algorithm for solving the visco-resistive equations of compressible magnetohydrodynamics. To solve the governing equations, a dealiased Fourier collocation method was used. Time was discretized by the modified Euler method, a second-order Runge-Kutta scheme. A parallel version of the code has been developed for the NRL CM-5, which permits resolutions of at least 256 x 256 x 256 Fourier modes.

Results: As a typical case, uniform twist, force-free fluxtubes were considered. The initial topology consisted of two orthogonal fluxtubes. This initial magnetic field distribution was then perturbed, permitting the fluxtubes to interact mutually and reconnect. Following a relatively quiescent phase, the fluxtubes were observed to reconnect explosively. A sheet of electric current formed between the two tubes from which a jet of magnetofluid was ejected at high speed.

Significance: The release of magnetic energy is thought to account for many phenomena in the solar atmosphere, such as flares and coronal heating. Our research on this complex system indicates that fluxtube reconnection is a plausible explanation for the hard X-ray bursts observed during two-ribbon flares. Predicting these bursts is crucial to advanced warning of DoD communication interruptions.



Several stages in the reconnection of two initially orthogonal, uniform twist, force-free magnetic fluxtubes. Magnetic field magnitude is shown with the isosurfaces chosen to have half the maximum magnitude at each stage.

Computational Chemistry and Materials Science

Computational Chemistry and Materials science encompasses a wide range of applications and computational techniques. The structures and properties of the smallest molecules and atoms are examined with advanced quantum mechanics while, on the other end of the spectrum, complex materials, such as metals and superconductors, are modeled with local density functional theory and molecular dynamics. CCM work is critical in designing new rocket propellants, explosives, structural and electronic materials, pharmaceuticals, and biomolecules. Calculations provide guidance to experimentalists that saves development time in all of these areas. The following eight success stories are prime examples of how the CCM area has affected DoD research.

Capt. Scott G. Wierschke
Phillips Laboratory
CTA Leader for CCM

Bond-Stretch Isomerism in Strained Organosilicon Compounds: An Application of Ab Initio Electronic Structure Theory

Jerry A. Boatz
Phillips Laboratory, Edwards Air Force Base, CA
Mark S. Gordon
Ames Laboratory - USDOE, Ames, IA

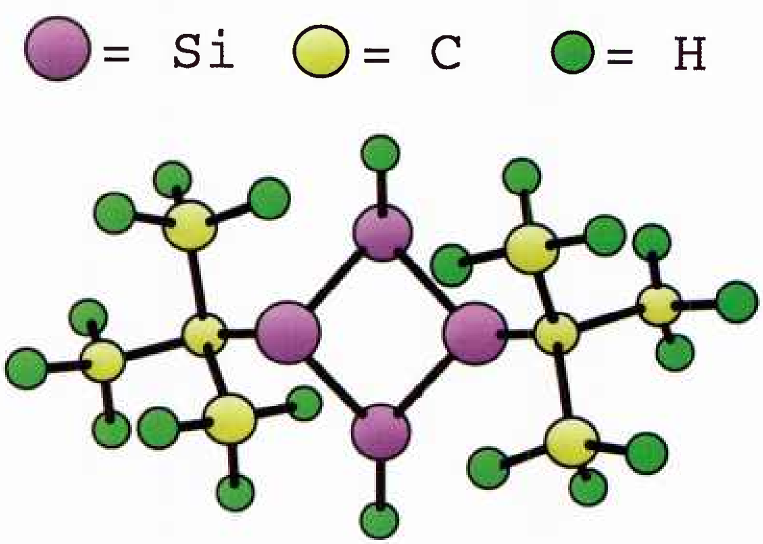
Computer Resource: Intel Touchstone Delta System [CalTech], local area network of IBM Risc/6000 workstations

Research Objective: To determine relative energies and isomerization barriers of the bond-stretch isomers of tetrasilabicyclo[1.1.0]butane (Si_4H_6) as a function of bridgehead substituents.

Methodology: A parallelized version of the ab initio electronic structure code GAMESS (General Atomic and Molecular Electronic Structure System) has been developed to run on a wide variety of parallel architectures, including both distributed and shared memory systems as well as clusters of workstations. The parallel version of GAMESS has enabled ab initio electronic structure theory to be applied to larger, more complex molecules. In the present work, GAMESS has been used to study the effects of varying the bridgehead substituents (-H, $-CH_3$, and $-C(CH_3)_3$) on the relative stabilities and isomerization barriers of Si_4H_6.

Results: The unsubstituted molecule Si_4H_6 is predicted to exist in two distinct "bicyclobutanelike" geometries, which differ primarily in the length of the Si-Si bridge bond. The local minimum with the longer bridge bond length (i.e., the "long-bond" isomer) is more stable than the short-bond counterpart by 10 kcal/molecule. Replacement of the bridgehead hydrogen atoms with methyl ($-CH_3$) groups reduces the energetic preference for the long-bond isomer to 2 kcal/molecule. Finally, placement of tertiary butyl groups ($-C(CH_3)_3$) at the bridgehead positions actually reverses the order of relative stability, with the short-bond isomer 5 kcal/molecule below the long-bond isomer in energy. The energetic preference for the short-bond structure with tertiary butyl groups at the bridgehead positions is consistent with the available experimental structural data on substituted tetrasila[1.1.0]bicyclobutane.

Significance: This work is being done in connection with the Air Force High Energy Density Matter Program, which seeks to identify, characterize, and exploit high-energy density systems for use as advanced rocket propellants. Preliminary calculations indicate that Si_4H_6, when used as an additive to LH_2/LOX propellants, is capable of improving specific impulse by up to 10 seconds, which would result in considerable savings in launch costs.



GVB/3-21G optimized geometry of the long-bond isomer of di-tert-butyltetrasilabicyclo[1.1.0]butane*

Nanocapillarity in Fullerene Tubules

Jeremy Q. Broughton and Mark R. Pederson
Naval Research Laboratory, Washington, DC

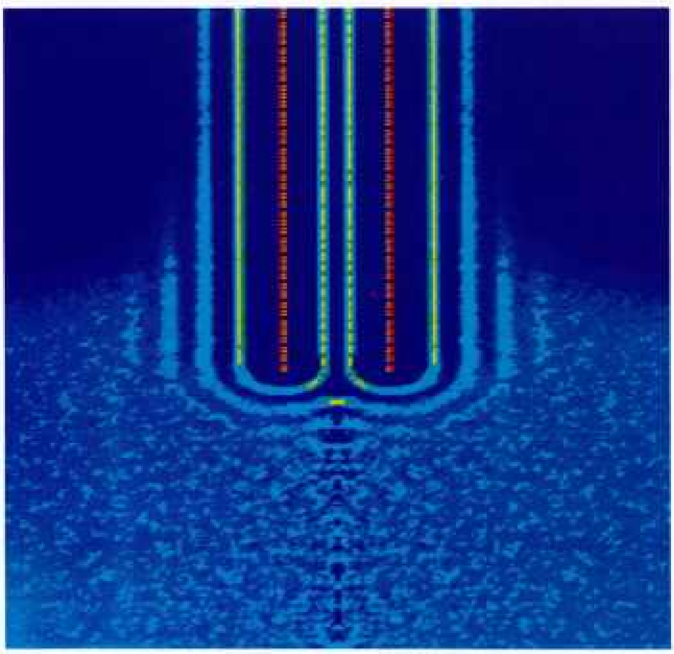
Computer Resource: Cray C-90 [CEWES, Vicksburg]

Research Objective: Soon after the discovery of the spherical fullerenes (e.g. C_{60}), it was found that similar tubule shaped structures could be obtained by arc-discharge between carbon tips. Although the tubules are presently produced with random orientation, control over their diameter is improving dramatically. Tubules are shaped like straws. We determined how strongly these “straws” can ingest—via capillarity—polar and nonpolar molecules.

Methodology: For polar ingestion, where we expected dipole induced-dipole interactions between the polarizable tubule perimeter and the dipolar molecule (e.g., H_2O), we used a local orbital density functional (LDA) code, which solved self-consistently the quantum mechanical Schrodinger equation for the system of electrons and nuclei. We moved a hydrogen-fluoride molecule from outside to inside a tubule of diameter 10 Å following the energy. For the nonpolar interaction, we used a statistical mechanical simulation method involving molecular dynamics and smart Monte Carlo to determine whether a representative fluid such as argon or neon would be entrapped in tubules of radii up to 20 Å. Such simulation methods allow systems to evolve to find their stable equilibrium state. We simulated tubules of 2000 carbon atoms and liquids of 20,000 atoms.

Results: The gaseous HF molecule was sucked towards the mouth of the tubule and ingested with an energy of 0.2 eV—easily enough to be absorbed at room temperature. The nonpolar fluids were all easily ingested, so much so that the “straw” completely filled itself and even continued to absorb significant amounts of the fluid on its outside.

Significance: Looking to the day when ordered arrays of tubules are available, fullerene tubules will make excellent storage devices for hydrogen and for absorbing pollutants. By tailoring their diameter, it is possible to make such systems selective for certain molecules—they will have novel catalytic uses. Pursuant to this work, tubules might be used for lubricant delivery in microscale machines. This theoretical work pre-empted experimental findings that corroborated our results. Energy storage, pollution control, and microminiaturization are all subjects crucial to DoD and U.S. competitiveness.



Longitudinal cut through tubule penetrating liquid neon surface. Red atoms denote carbons. Dark blue to light blue to yellow represents increasing density of Ne.

Nonlinear Optical Materials in Solution

Paul Day and Ruth Pachter
Wright Laboratory, Wright-Patterson Air Force Base, OH

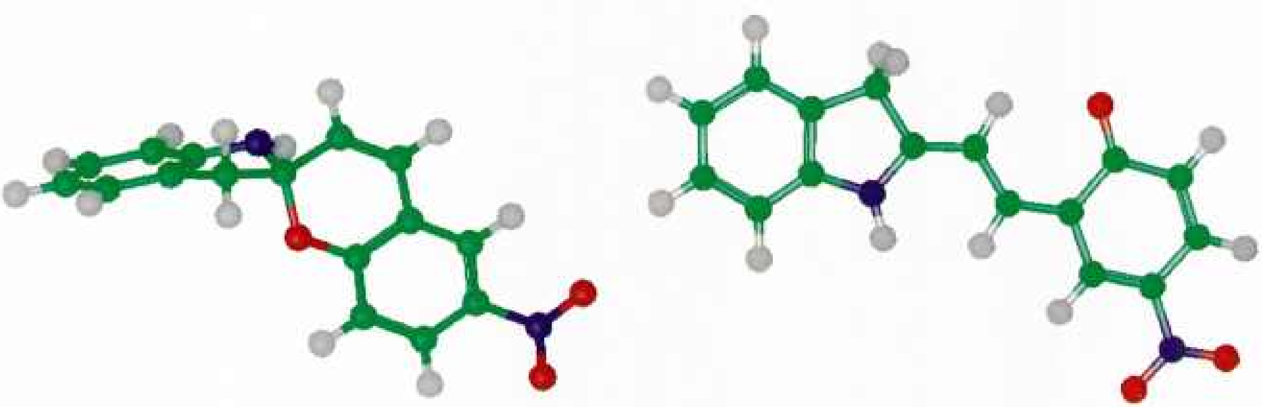
Computer Resource: Intel Paragon XP/S-15 [ASC, Wright-Patterson AFB, OH] and Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: The evaluation of nonlinear optical properties and reaction energetics in the presence of solvent is essential to develop materials for optical limiting and optical switches. In particular, the reaction energetics and properties of pyran and nitrochromene, used as models for the ring-opening of spiropyran to merocyanine, were studied to gain an understanding of solvent effects. Such extensive ab initio quantum mechanical calculations require new methods and scalable high performance computing.

Methodology: The effective fragment potential (EFP) approach was developed to include solvent effects in ab initio calculations and was incorporated in the GAMESS program with the routines for calculating the solvent effects being parallelized. In the EFP method, intermolecular interactions are taken into account using electrostatic, polarizability, and exchange repulsion terms, where the development of the polarizability energy model was an important part of the approach.

Results: The ring-opening reaction of pyran has been studied in detail, revealing an incorrect previous study of this reaction. The inclusion of microsolvation and bulk solvation indicates a large effect on the nonlinear optical properties. Indeed, the effective fragment potential approach, which allows for a more realistic simulation of solvent, is critical in the evaluation of such properties of materials in solution. The need for parallel computing in carrying out these ab initio calculations was clearly demonstrated. For example, a comparison of the performance in using GAMESS with a 3-21G basis (229 basis functions) indicates that 30 processors on the Paragon are over three times as fast as a single processor on the Cray C-90. The speed-up when changing from 60 to 90 processors is about 1.4 for a larger 6-31G(d) basis set for spiropyran (339 basis functions), or about 91% efficient. Such a calculation is not feasible on the Cray C-90.

Significance: The development of a realistic modeling methodology to be used in molecular design studies of new materials is enabled by the inclusion of solvation effects for properties calculations from first principles, as is being developed within parallel GAMESS. Indeed, the derivation of such an approach would impact the scientific community in general for any materials development, including biomaterials, as well as in the design of novel nonlinear optical materials that are essential for the DoD mission, particularly for optical limiting and optical switches.



The ring-opening reaction of spiropyran (left) to form merocyanine (right)

HPC Material Design: Assembled Nanostructured Materials

Ryoichi Kawai
University of Alabama, Birmingham, AL
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University of California San Diego, La Jolla, CA
Office of Naval Research, Arlington, VA

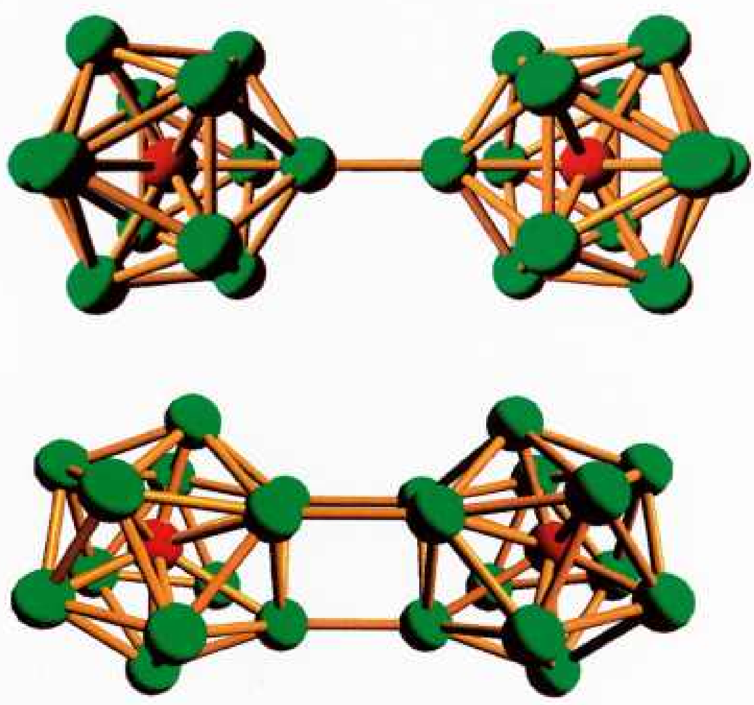
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS] and TMC CM-5E and CM-200 [NRL, Washington, DC]

Research Objective: To investigate the problems associated with the assembly of new bulk materials from nanoscale metal clusters with unique properties.

Methodology: In these systems, the bonding is very nondirectional and delocalized. Methods based directly on the solution to the electronic Schrodinger equation are required to calculate the interactions between atoms. Our methods are based on plane wave expansions of the local density approximation (LDA). Because the systems are so large, very efficient methods to handle the large structured matrix operations that are required (such as multiplication and eigen values) must be found and implemented on massively parallel computers.

Results: Interesting and unexpected bonding patterns have been found in highly unsaturated simple metal clusters. In addition, these systems show remarkable stability for certain particle sizes. This correlates well with the filling of shells of a simple jellium model. Our calculations have shown that we can produce materials with very high stability by adding electrons to produce filled jellium shells, as in $Al_{12}C$. These materials have a very large HUMO-LUMO gap and are therefore quite stable. We have shown that they have potentially important properties such as high polarizability. However, even these clusters have appreciable interaction when placed at separations typical of the bulk.

Significance: The next generation of electronic devices will require the ability to control placement and positioning of electronically active materials at resolutions of 10 nm or better, in order to reach the information density and speed required in future defense applications. This line of research on the factors governing the formation of regular nanometer-scale structures serves to disclose the basic rules by which such structures can be manipulated in a fabrication scheme.



Structure of $Al_{12}C$ dimers: (top) vertex bonding; (bottom) face bonding

Low-Energy Phenomena in Clusters and Cluster-Assembled Materials

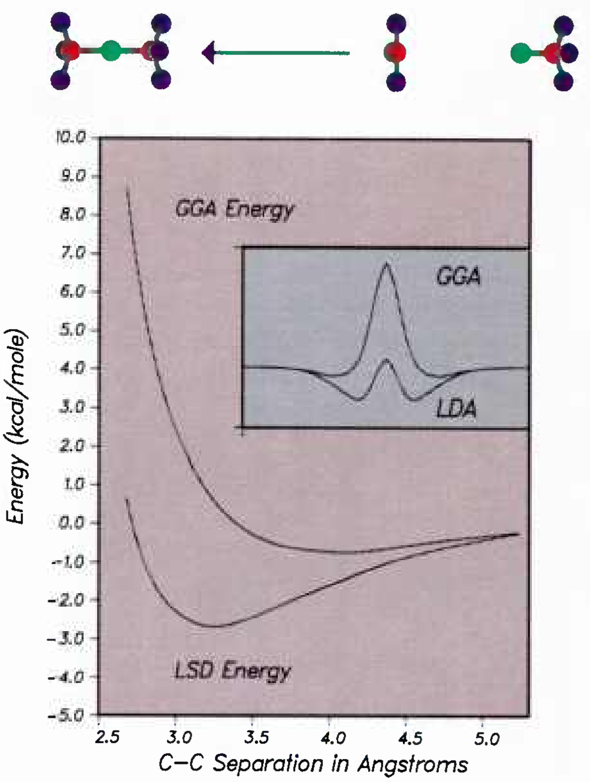
Mark R. Pederson
Naval Research Laboratory, Washington, DC

Computer Resource: Cray C-90 and Cray Y-MP [CEWES, Vicksburg, MS]

Research Objective: To expand the applicability of density-functional based methods to study clusters, cluster assemblies, and nanoscale systems and to perform calculations that are of current interest to the field of clusters and cluster assemblies.

Methodology: We used the all-electron, Gaussian-based density-functional codes of Pederson et al. to calculate the electronic and vibrational spectrum, total and cohesive energies, interatomic forces, and other phenomena of interest.

Results: Density-functional-based calculations of the methyl-methane hydrogen exchange reaction energy have been performed. Previously, reaction barriers could not be calculated with efficient density-functional methods because of the overbinding in the local density approximation (LDA). In contrast, within the generalized gradient approximation (GGA), the 0.1 eV/atom errors in the cohesive energies are approximately five times smaller than most reaction barriers. The hydrogen exchange reaction between a methyl radical and a methane molecule provides a well-understood test case. We find that while the LDA predicts no reaction barrier, the GGA predicts a barrier of 9 to 13 kcal/mole, which agrees well with the experimentally observed barrier of 14 kcal/mole. This work will soon be appearing in Chemical Physics Letters. To address recent experimental reports, which suggest that fullerene molecules can form dimers and long-chain polymers, large-scale calculations on the 120-atom fullerene dimer have been performed. The dimer is found to be stable with a cohesive energy and geometry that is in excellent accord with experimental measurements. The fullerene molecules polymerize with extremely short center-to-center distances. Also, the calculations show that the observed changes in the infrared vibrational spectrum are primarily due to on-ball changes of the dynamical matrix.



Significance: This work shows that reaction rates can be reliably predicted given several hundred hours of supercomputer time using efficient implementation of the GGA. The next step will be the study of catalytic pathways (and how to improve them) on surfaces using periodic codes; such pathways have been heretofore intractable. The work on the fullerenes resolved experimental ambiguities in their vibrational characterization. All in all, LDA and GGA are powerful complements to experiments in, and have impressive predictive abilities for, DoD technology and the U.S. chemical industry.

The energy barrier of a CH_3-CH_4 complex as calculated within the old (LDA) and new improved (GGA) versions of density-functional theory. The GGA energy barrier is in good agreement with experimental findings, which suggests that a density-functional-based description of reaction rates and catalysis is possible.

A Diamond-based Electron-emitting Surface

Warren E. Pickett
Naval Research Laboratory, Washington, DC

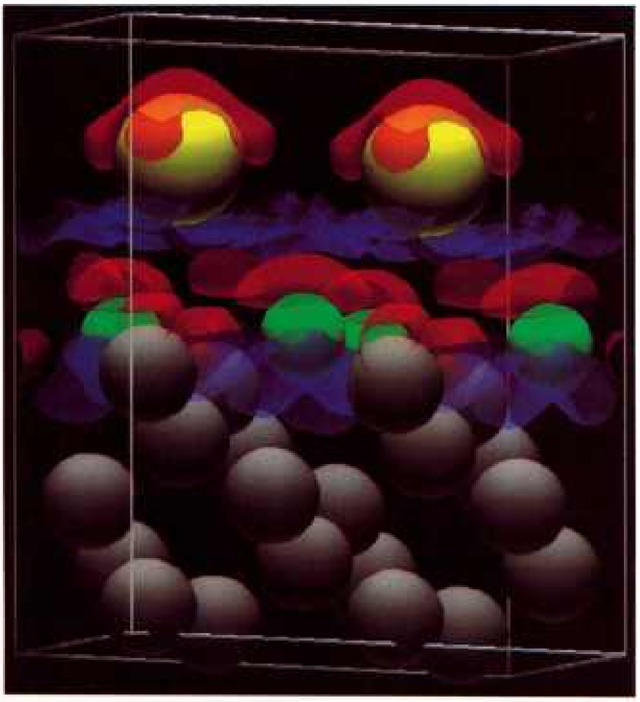
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: Surfaces that can be induced to emit electrons easily have numerous applications, from photomultipliers for night vision goggles, to long-lived unheated photocathodes suitable for satellite components, to flat panel displays for DoD systems and for high definition TV. Our aim is to determine whether diamond can be used as the basic material, thereby providing more strength, high temperature stability, and laser hardness than conventional semiconductors. Diamond's wide bandgap would also provide operation in higher frequency ranges than is presently possible.

Methodology: The atomic geometry and electronic properties of surfaces can be obtained by using the density-functional-based FLAPW code, which solves self-consistently the quantum mechanical Schrodinger equation for electrons in the presence of nuclei. The FLAPW codes expand the electronic wavefunctions in basis sets and solve the resulting linear equations. This system leads to matrix equations of order 3800 x 3800, making the very large memory of the Cray C-90 essential for this study. Based on analogy with metal-based cold cathodes presently in use, the choice of system for study was a (100) surface of diamond, first oxygenated to eliminate the electrical activity of dangling electronic bonds, then covered with cesium at the half monolayer level to induce a large electronic surface dipole.

Results: The calculation shows that this combination will behave as a negative electronic affinity (NEA) device, i.e., electrons excited into the conduction bands (by light, by electric fields, or even thermally in doped material) will be spontaneously emitted from the surface. This highly desirable property is the result of charge transfer and electron rebonding within a 10-Å layer at the surface.

Significance: Diamond-based emitter arrays are being pursued both in the United States and in Japan. This calculation provides an interpretation of a recent result from MIT Lincoln Labs, in which a related but uncharacterized cesium-on-oxygenated diamond surface showed not only favorable field emission current densities but remarkable stability as well. Calculated energies suggest that this proposed surface is relatively stable. Experimental verification that this is in fact an NEA surface will open the possibility of many new optoelectronic applications based on diamond substrates. An additional feature is that this system has a subnanometer-thick metallic region at the surface that can be used to drain charge that would otherwise rapidly block device operation. A working NEA device such as this promises to be could strongly impact applications both in the military (e.g. image intensifiers, space-based electronics) and in industry (HDTV, coatings for photocathodes).



Atomic positions for this NEA system: carbon—light gray; oxygen—green; cesium—blue. Red and yellow surfaces indicate regions of charge buildup and depletion, respectively, that result in formation of a large surface dipole.

Shock and Detonation

Betsy M. Rice, John Grosh, and Michael J. Unekis
U.S. Army Research Laboratory, Aberdeen Proving Ground, MD

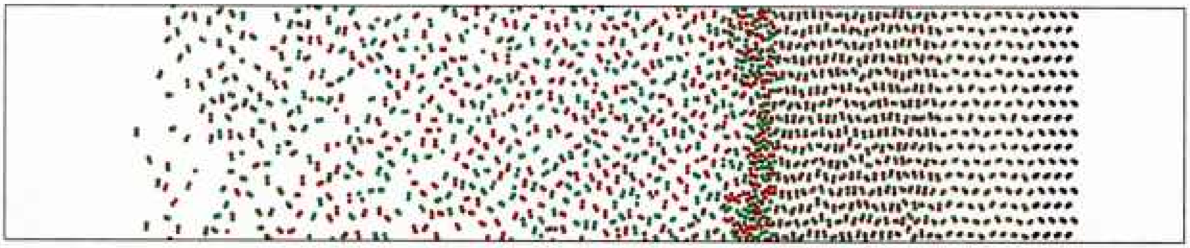
Computer Resource: Cray Y-MP and C-90 [CEWES, Vicksburg, MS]

Research Objective: To determine, through classical mechanical simulation, why exceptionally powerful explosions occur in solid energetic materials under conditions of high pressure plus shear deformation (HP + SD).

Methodology: Working equations for the simulation are Newton's equations of motion ($F = ma$) transformed to Hamilton's equations, which are first-order ordinary differential equations. The integrator is a variable-step Adams-Moulton fourth-order predictor-corrector.

Results: We calculated shock/detonation for standard conditions and for the crystal under high uniaxial stress. The figure shows four well-behaved zones in the crystal, separated by three shock fronts. Shock profiles of the crystal under high uniaxial stress do not resemble those of this figure. There is significant instability in the shock fronts, caused by the reorientation and pressure-induced reaction of molecules due to the high-stress condition. This work will be published in the *Proceedings of the 1994 Army Science Conference.*

Significance: Determining the cause of an HP + SD explosion provides the knowledge necessary to manipulate the chemical and physical properties of explosives so that lethality is enhanced while protection of the soldier and equipment is maximized during use and handling. Additionally, innovative data reduction methods developed for convenient evaluation of the massive data sets generated by these simulations can be used for extraction and processing of immense data sets. Optimization and parallelization strategies have also been developed that can be readily applied to a wide variety of calculations.



Snapshot of detonating energetic crystal under standard conditions

HPC Material Design: Nanoscale Carbon Materials

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University of California San Diego, La Jolla, CA
R. Kawai
University of Alabama, Birmingham, AL
Office of Naval Research, Arlington, VA

Computer Resource: TMC CM-5 [AHPCRC, Minneapolis, MN]; TMC CM-5E and CM-200 [NRL, Washington, DC] and Kendall Square Research KSR1 [ARL, Aberdeen Proving Ground, MD]

Research Objective: To calculate the electronic structure and reactivity (e.g., degradation and growth) of nanoscale carbon materials using first-principles simulations.

Methodology: Because of bond breaking, the electronic Schrodinger equation must be solved to obtain atomic forces. We use ab initio molecular dynamics, which is based on the local density approximation. However, for carbon and oxygen (often responsible for degradation), the pseudopotentials are very strong, implying that plane basis sets must be very large. By implementation on parallel computers, we have obtained the significant speedups necessary to simulate large systems.

Results: The pentagonal/hexagonal fullerene structures are present in most nanosized carbon materials. The smallest closed fullerene is the C_{20} molecule. Our calculations show that, contrary to experimental results and prior calculations, this structure is considerably lower in energy than other structures such as the ring. The planar bowl (corranulenelike) structure and the fullerene are nearly degenerate. Other results show that the electronic structure of pure carbon ring compounds is similar to materials, such as polyacetylene, that possess strong nonlinear optical behavior. However, the band gap state, which is responsible for the optical behavior, is less localized than would be expected from current more approximate theories. As shown below, carbon melts to stringlike structures rather than unstructured liquids as in metals. This may explain the difficulty of getting good equilibration in gas phase synthesis.

Significance: This research is likely to lead to new methods of fabricating strong lightweight materials that are required in the DoD of tomorrow to reduce costs and fuel expenditure in vehicles and to provide better protective armor. Development of future manufacturing technologies will require the detailed understanding at the molecular level that this research provides.

Thermal decomposition of C_{20} fullerene: (left) T = 0 K; (center) intermediate T; (right) final melted structure

Computational Electromagnetics and Acoustics

In the technical area of Computational Electromagnetics and Acoustics, simulating time-domain signature and radiating phenomena by solving the multi-dimensional Maxwell equations with either a ray-tracing or a time-dependent, finite-volume numerical procedure represents the state-of-the-art. Predictive capabilities for long-range acoustic propagation in inhomogeneous media across a vortex shedding wake and a scattered acoustic field from a penetrable interface are also highlighted. Finally, interdisciplinary magnetohydrodynamic simulations of a solar chromospheric eruption, a laser-plasma accelerator, as well as space debris and nuclear weapons investigations clearly illustrate the wide range of applicability of HPC to the DoD mission.

Dr. Joseph J. S. Shang
Wright Laboratory
CTA Leader for CEA

Aerospace Noncooperative Target Recognition Program

Maj. Dennis J. Andersh, U.S. Air Force
Wright Laboratory, Wright-Patterson Air Force Base, Ohio

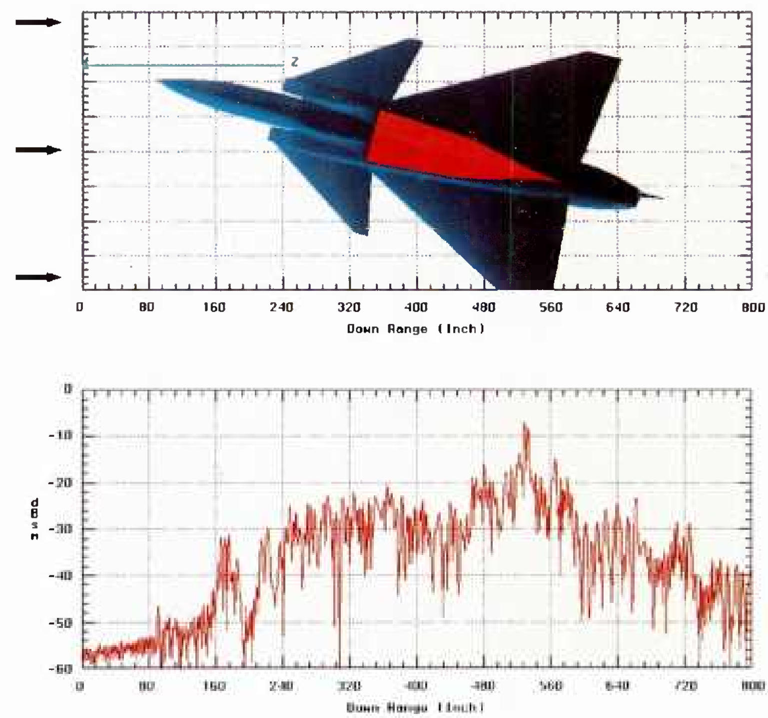
Computer Resource: Intel Paragon XP/S-25 [NRaD, San Diego, CA]

Research Objective: The primary objective of the Aerospace Noncooperative Target Recognition (NCTR) Program is to develop automatic target recognition algorithms and processing hardware capable of positively identifying threat, neutral, and friendly aircraft and ground vehicles. Accurate radar signature prediction codes and geometry descriptions are a requirement because predicted radar signatures are used as templates in the identification algorithms.

Methodology: One of the most significant technology development efforts being jointly conducted by Wright Laboratory, Massachusetts Institute of Technology/Lincoln Laboratory, Sandia National Laboratories, the Naval Air Warfare Center, Army Research Laboratory, and 15 other university and industry organizations involves the development of UHF through Ka band, full target in scene, electromagnetic (EM) prediction codes. The EM prediction codes are fully polarimetric, and they handle perfect electric conducting material, homogeneous and isotropic frequency-dependent materials, radar-absorbing nets, and materials such as fiberglass and other semitransparent materials. The synthetic signature prediction effort uses computer-aided design (CAD) files as the basis of the description of the target geometries. Sandia National Laboratories is hosting the radar prediction codes on several massively parallel machines. However, almost all of our prediction work is classified SECRET or higher, which limits dedicated production at Sandia to a single classified 64-node Intel Hypercube.

Results: This work was recently ported from Sandia to the Intel Paragon at NRaD where radar signature production is performed on the 300+ node machine 24 hours around the clock. This has allowed the recovery of a 5-month deficit of continuous computations in about 1 month and avoided a potential loss of $2M to $3M in development costs on a very time-critical program. With today's computational technology, we will be required to run 24 hours around the clock for several years to compile the more than 10 million signatures and images required for NCTR development and operational fielding. We plan to continue using the HPC asset at NRaD over the next 2 to 5 years as well as other classified high performance computer assets as they become available.

Significance: The NCTR technology is one of the critical technology areas as demonstrated by the recent inadvertent shoot-down of helicopters in Iraq. The signature prediction technology is also being used in wireless communication system designs and in remote sensing projects to detect hazardous waste and unexploded ordnance.



Computer-predicted time domain signature

Coupled Seismic Waves

Stanley A. Chin-Bing and David B. King
Naval Research Laboratory, Stennis Space Center, MS

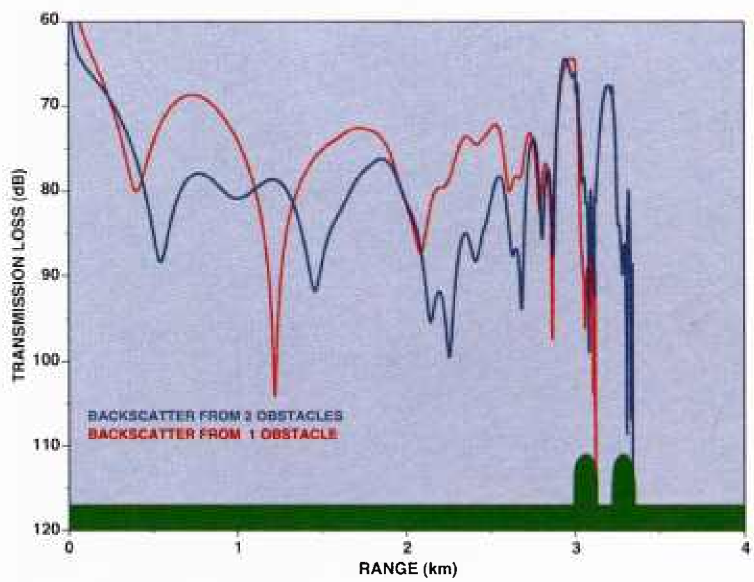
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS] and Cray M-98 [ARSC, Fairbanks, AK]

Research Objective: By using computer simulations, to develop the capability to predict the effects of shear and compressional wave mode coupling on long-range acoustic propagation and scattering in shallow-water, range-dependent ocean environments; to identify the effects of long-range shear conversion on ocean acoustic propagation and reverberation; and to analyze the Office of Naval Research's Acoustic Reverberation Special Research Program (ONR ARSRP) data.

Methodology: The finite-element method was used to solve the inhomogeneous anelastic Helmholtz wave equation (including the acoustic source function) for inhomogeneous media. Both coupled two-dimensional Helmholtz wave equations (acoustic and elastic) were solved by using a noniterative inversion of nonsparse matrices with complex elements. Matrix elements are complex, because of the "true" (as opposed to adiabatic) way of including compression and shear wave attenuations, and nonsymmetric, because of the mathematical representations of radiation boundary conditions. Three ocean-acoustic computer models were used: FOAM, FFRAME, and SAFE. The computer codes are amenable to some vector processing. Each was combined with a parabolic equation (PE) model to form hybrid models with more capability. The PE model has been fully vectorized.

Results: These finite-element models together with several other highly accurate ocean acoustic computer models were used to generate reference solutions for an ONR-sponsored workshop: the Reverberation and Scattering Workshop, 3-5 May 1994, Gulfport, MS. More than a dozen reference solutions were generated for this workshop. Each represented a state-of-the-art result in acoustic backscattering, each and was used to determine the accuracy of other ocean reverberation computer models. The figure compares computer-simulated acoustic backscatter (in the form of transmission loss) from one and two seafloor obstructions (shown in green at the bottom of the figure).

Significance: The use of computationally intensive, benchmark-accurate, ocean acoustic frequency-domain models to produce time-domain results is a first; it could only have been accomplished through this HPC grant. Results from the Reverberation and Scattering Workshop will be published by the Naval Research Laboratory. The reference solutions represent the standard against which future ocean acoustic reverberation models will be compared.



Reference solution from ONR Reverberation Workshop; backscattered energy from one and two round top obstacles (shown in green)

Shallow Water Fluctuations

Stanley A. Chin-Bing and David B. King
Naval Research Laboratory, Stennis Space Center, MS

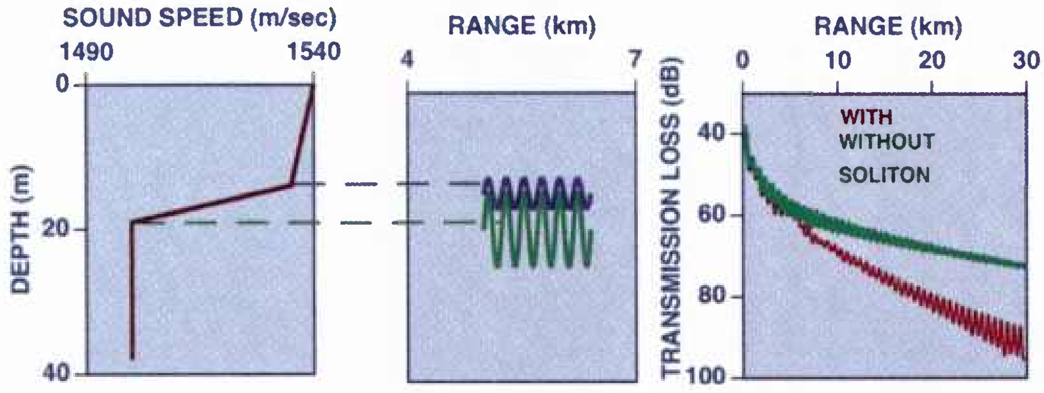
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: To determine long-range ocean acoustic effects (e.g., mode conversion) resulting from fluctuating environmental features in a shallow-water environment, to identify the physical mechanisms that cause these effects, and to develop a predictive capability that includes the effects (viz., develop a stochastic-statistical propagation model that includes random media effects).

Methodology: Highly accurate ocean acoustic computer models were used to identify important mechanisms that affect shallow-water acoustic propagation through fluctuating media. The models applied were those developed in the subproject "Coupled Seismic Waves." These models are full-wave, range-dependent, coupled two-way, finite-element models (FOAM, FFRAME, SAFE); they were verified to be benchmark accurate in their acoustic predictions. Emphasis will be on determining mode conversions and resonances that occur as a result of environmental fluctuations in shallow water. All shallow-water boundaries will be included in the simulation because the shallow-water waveguide extends from the sea surface to the ocean subbottom and "molds" the incident wave field that interacts with the fluctuating media. Once the important physical mechanisms of the fluctuating media are determined and quantified, they will be included in the development of a shallow-water average propagation acoustic model. Verifications will be made by comparing with experimental and synthetic data and by using ensemble averages from a large number of deterministic computer runs.

Results: Resonance effects in shallow-water internal waves (solitons) have been simulated by using highly accurate ocean acoustic computer models. This resonance effect occurs only at certain frequencies and is strongly coupled with ocean bottom attenuation. We have shown that this effect is dependent on the spatial extent of the soliton and can occur for a single soliton wave packet. The figures show the sharp discontinuity in ocean sound speed along the thermocline, the simulated soliton, and the resulting effects of the soliton on the transmission loss.

Significance: Two significant advances have been made as a result of these model simulations. First, the resonance effect has been shown to occur for a single internal wave packet; prior to this simulation, it was believed that several wave packets were needed. Second, internal waves are now a viable explanation of the anomalous results observed in recent data. Until this work, fish schools were considered to be the only plausible explanation.



Shallow-water sound speed profile

Effect on sound speed caused by passing of soliton

Acoustic resonance effect of soliton

Acoustic Boundary Characterization (Fractal Acoustics)

Stanley A. Chin-Bing
Naval Research Laboratory, Stennis Space Center, MS

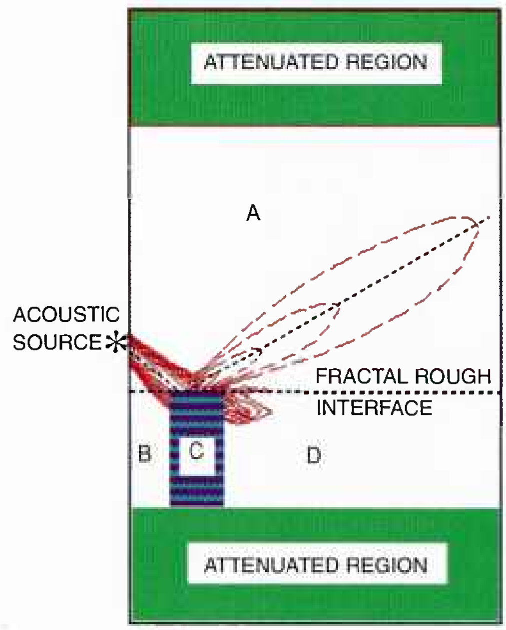
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: To determine if the rough, penetrable seafloor (i.e., the rough seafloor and its subsurface composition) is fractal-like in its acoustic response and to quantify the limits of this "diffractal" seafloor roughness. From this knowledge, methods will be developed for generating acoustically valid, equivalent sea floor "acoustic roughness" simulations. This project will use computer simulations to determine if seafloor roughness and subsurface composition combine to produce fractal-like acoustic responses.

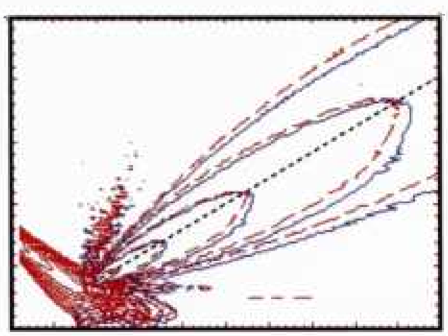
Methodology: Benchmark accurate acoustic numerical models, together with representations of seafloor surface roughness and subsurface composition were used to generate simulated scattered acoustic fields, which were analyzed to determine if they are "diffractal" and thus enable the combination of surface roughness and subsurface composition to be characterized as fractal, multi-fractal, or nonfractal for chosen acoustic bandwidths. Shear wave seismoacoustic models were used to determine the effect of the subbottom underlying the fractal interface.

Results: Computer codes have been developed to create acoustically penetrable, band-limited fractal surfaces. Computer simulations of acoustic scatter off the fractal surfaces and through the fractal surfaces were made by using the FFRAME and SAFE models. The figures below illustrate the method and some results. The figure on the left illustrates the "numerical experiment." Region C is the penetrable ocean bottom. It is isolated by surrounding regions A, B, and D. The rough, penetrable fractal bottom is on top of region C. Attenuated regions are placed at the very top and bottom to prevent nonphysical reflections. Computer simulations show that the diffracted acoustic fields from these penetrable fractal surfaces were affected by the properties of the underlying penetrable material. The diffracted fields exhibited fractal structure when the acoustic frequencies were within the fractal part of the bandwidth. No correlated effects were seen when the acoustic frequencies were outside the fractal part of the bandwidth. Results are illustrated in the figure on the right. The red and blue curves differ as the result of the penetrable subbottom region, i.e., region C shown in the left figure.

Significance: Computer simulations have demonstrated that the material composition underlying a fractal surface can affect the scattered acoustic field to the extent that what is considered to be a fractal surface may not be acoustically fractal. This has significant implications on ocean bottom-seafloor descriptions used in underwater acoustic detection and classification systems. Inaccurate descriptions can produce false detections.



Schematic of numerical experiment



Acoustic field results

Magnetic Reconnection in Chromospheric Eruptions

J. T. Karpen, S. K. Antiochos, and C. R. DeVore
Naval Research Laboratory, Washington, DC

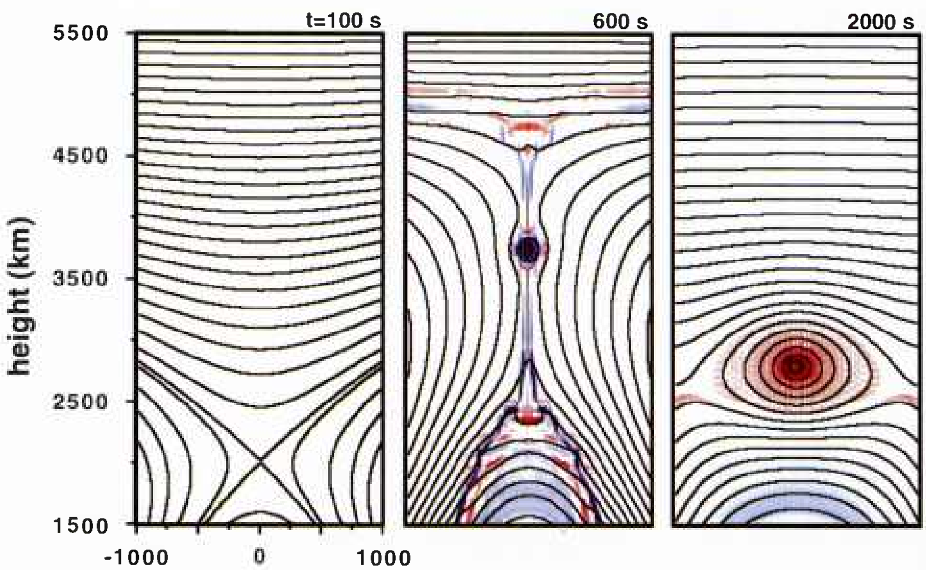
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: Several solar phenomena observed in a variety of spectral regimes have been classified as chromospheric eruptions (CEs); these include spicules, surges, sprays, explosive events, and microflares. Although the various types of CEs are not identical, the underlying physics appears to be similar. Observations imply that the explosive events are caused by magnetic reconnection in emerging flux regions and at the edges of the network. Hence, the primary question is whether reconnection in chromospheric conditions can explain the observed properties of CEs.

Methodology: This study was focused on modeling shear-driven magnetic reconnection in the solar chromosphere. The calculations were performed with MAG25D, our 2.5-dimensional finite-difference code that solves the compressible, time-dependent conservation equations of ideal magnetohydrodynamics via flux-corrected transport algorithms. Our simulations began with a potential magnetic 2-D field containing a central X point at a height of 2000 km, embedded in a model chromosphere with solar gravity and numerical resistivity. A series of runs were performed with varying numerical resistivity and shear strength; each run used about 10 to 20 CPU hours.

Results: For a strong localized shear, the X point begins to lengthen into a current sheet (CS) and reconnection starts around 300 s. After 400 s, several magnetic islands develop in sequence, move towards the extremities of the CS, and eventually disappear through reconnection with the overlying or underlying field. The presence of oppositely directed flows is consistent with spectroscopic observations of many CEs. Finally, a new quasi-equilibrium state arises with a central magnetic island a few hundred km above the site of the initial X point. We conclude that magnetic reconnection can account for the plasma dynamics observed in CEs. A paper describing these results will appear in the *Astrophysical Journal.*

Significance: These are the first simulations of shear-driven reconnection in a realistic solar atmosphere, a process fundamental to most solar activity including flares, coronal heating, and coronal mass injections. By increasing our understanding of the genesis of CEs, we enhance the Navy's ability to predict solar activity affecting vital communications, spacecraft operations, and the commercial power grid.



Magnetic field (black lines) and electric current (color) in the reconnection region

Control of Acoustics in Cylinder Wake Flows by Wall Heating/Cooling

T. S. Mautner and D. S. Park
Naval Command, Control and Ocean Surveillance Center, San Diego, CA

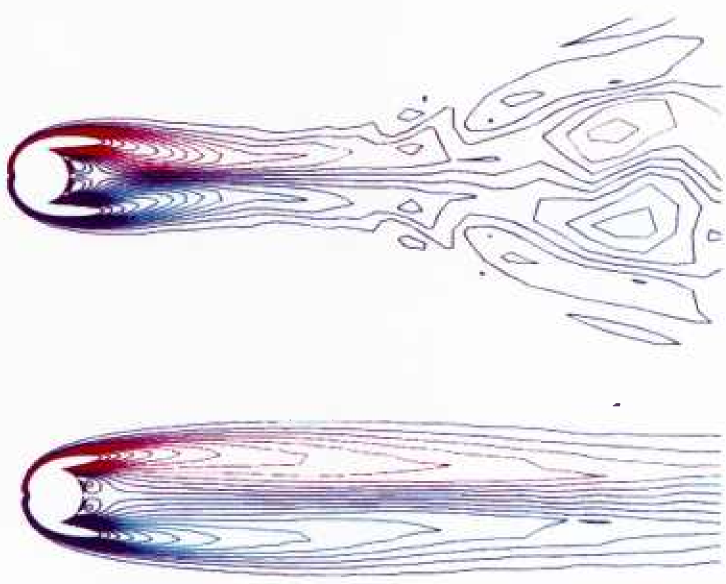
Computer Resource: Cray M-98 [ARSC, Fairbanks, AK] and Cray Y-MP [CEWES, Vicksburg, MS]

Research Objective: To develop a feedback mechanism to control the acoustic signature of a cylinder undergoing vortex shedding. This is accomplished by manipulating various temperature distributions on the cylinder surface and computing the resulting time-dependent flowfield and radiated sound field.

Methodology: The two-dimensional time-dependent, incompressible flow past a circular cylinder was computed by using an explicit finite-difference representation of the Navier-Stokes equations in vorticity-stream function form coupled with the scalar transport equation for temperature. The usual boundary conditions were modified to contain a wall temperature profile $T = -g(t) \sin 2\theta$, which is a function of angular position θ and gain $g(t)$ determined by the feedback mechanism. The results of flow-field calculations were then used to compute the low Mach number sound field by using a low-frequency Green's function approach.

Results: Complete suppression of cylinder vortex shedding can be achieved by constant wall heating of sufficient magnitude. However, if the amount of heat input is also dependent on the magnitude of the vortex shedding, the overall heat requirement can be minimized. The computational results show that, for various Reynolds numbers (Re = ratio of inertia and viscous forces) and Grashoff numbers (Gr = ratio of buoyancy and viscous forces), the anti-symmetrical wall heating adjusted by the time-dependent gain function can reduce and/or suppress vortex shedding. The computed acoustic signature magnitude also reflects the reduction in radiated sound [T.S. Mautner and D.S. Park, "Control of Acoustics in Cylinder Wake Flows by Wall Heating/Cooling," presented at International Mechanical Engineering Congress and Expositions, Chicago, IL, Nov. 1994].

Significance: An effective method of vortex shedding and acoustic control, at low Reynolds numbers, has been developed. The developed theory and numerical experiments demonstrate the ability of a simple feedback control system to modify the mean flow using a minimum amount of surface heating. This system can be modified to an internal system using surface properties and to one that can operate at higher Reynolds numbers. The system's simplicity makes it easily applied to existing arrays, cables, etc. for both stabilization and acoustic control. It can also be designed and evaluated via numerical experiments.



Isovorticity contours for a feedback-controlled case with Gr/Re2 = *6. (top)* $t = 50$*, (bottom)* $t = 100$*, after heat is turned on*

Quasi-static Particle Model of a Laser-Plasma Accelerator

Jonathan Krall, Phillip Sprangle, Eric Esarey, and Glenn Joyce
Naval Research Laboratory, Washington, DC

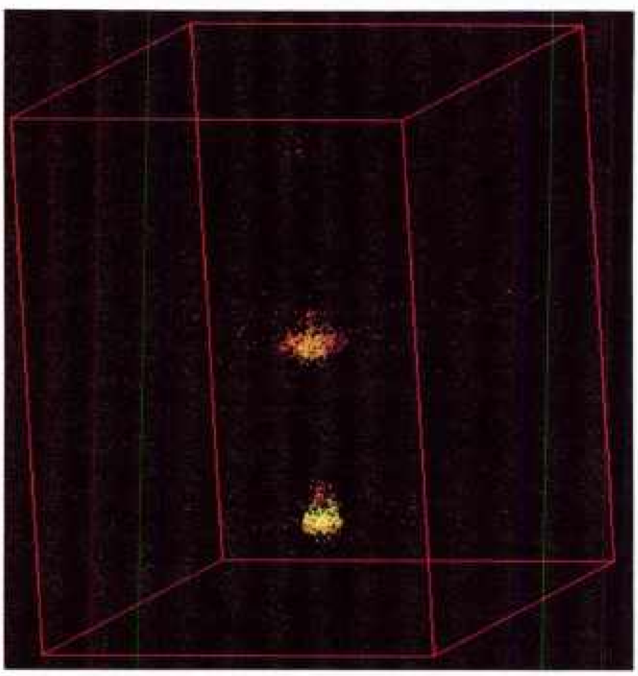
Computer Resource: TMC CM-5 [NRL, Washington, DC]

Research Objective: To design next-generation accelerators, an understanding of laser propagation in a plasma is needed. A currently planned experiment at the Naval Research Laboratory (NRL) will test the self-modulated laser wake-field accelerator (SM-LWFA) concept. In the SM-LWFA, a high-intensity laser pulse excites an electrostatic wave in a plasma (an ionized gas). The large electric field of the plasma wave can accelerate electrons to high energies. This is an alternative to the laser-plasma accelerator being tested at the University of California Los Angeles [*New York Times*, 4/19/94].

Methodology: The laser interaction-laser acceleration (LILA) code takes advantage of the separation between the short laser scale length (microns) and the long plasma scale length (millimeters). This allows the quasi-static electromagnetic fields to be "frozen" while the particles are pushed in parallel on the CM-5. The amount of time spent solving for the fields and the number of particles are reduced. LILA is an extension of the workstation-based, laser-electromagnetic (LEM), quasi-static fluid code.

Results: LILA is up and running and, along with the LEM code, has been used to simulate the planned NRL SM-LWFA experiment; results are shown here. Three accelerated electron bunches (moving towards the right) can be seen; color coding indicates the electron energy. With yellow indicating energy greater than 50 MeV and bright yellow indicating 100 MeV, this shows 100 MeV acceleration in 1 mm. This is a factor of 1000 beyond conventional accelerator technology, such as that used in the Stanford linear collider (SLC), the superconducting supercollider (SSC), and the European large hadron collider (LHC).

Significance: The increase in accelerating gradient quoted above implies a 1000-fold reduction in the length of the accelerator needed to produce a given particle energy. Ultimately, a future SLC or SSC-type accelerator might be replaced by a plasma-based accelerator—doing the same job with significantly less real estate and concrete. Reducing the cost of such accelerators will also increase their availability, opening new doors in DoD weapons, medical, and materials-processing research.



Particle plot of trapped electrons in the laser wake-field accelerator

Scattered Electromagnetic Field of a Reentry Vehicle

J.S. Shang and D. Gaitonde
Wright Laboratory, Wright-Patterson Air Force Base, OH

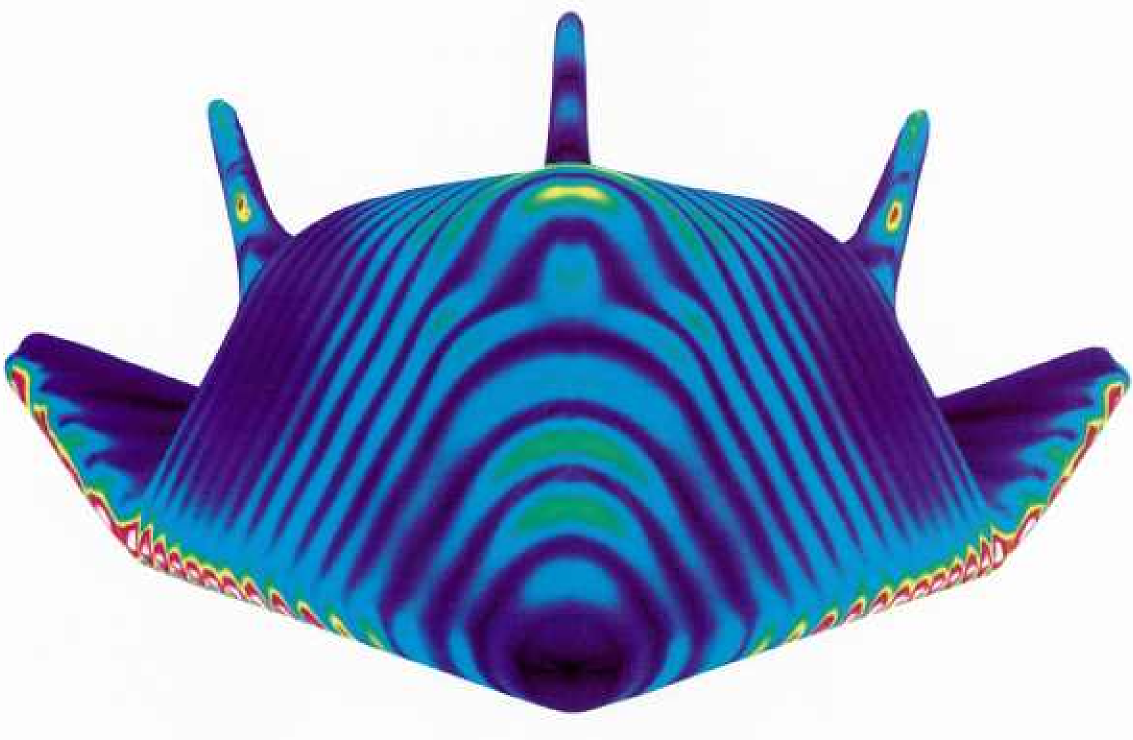
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS] and Intel Paragon XP/S 240 [Wright-Patterson AFB, OH]

Research Objective: To create an efficient and scalable numerical capability to solve the three-dimensional Maxwell equations in the time domain for electromagnetic phenomena. To develop the electromagnetic and acoustic signature simulation technology for surveillance, communication, microwave, biological, and dual-use applications.

Methodology: A characteristic-based, flux differencing, finite-volume algorithm was adapted to solve the time-dependent, 3-D Maxwell equations. Consistent numerical accuracy in time was obtained by a Runge-Kutta family of single-step, two-stage procedures. For concurrent computations, the high numerical efficiency was derived from a simple yet effective 1-D domain decomposition strategy.

Results: The numerical results were first verified by comparing them with benchmark data of an infinite cylinder and an oscillating electric dipole. The radar cross section (RCS) of a scaled X24C-10D re-entry vehicle was then obtained in the optical regime, where the vehicle length to the illuminating wavelength had a ratio of 9.3. The numerical procedure has achieved a data processing rate of 570 Mflops on a single processor of a Cray C916/16256 system for an RCS calculation. Mapping onto the 512-node Intel Touchstone Delta system, the data processing rate of this code exceeded 5.96 Gflops.

Significance: The newly developed numerical simulation provides the capability for faultless target identification and signature prediction for defense. This technique can be applied equally well to high-performance antenna design and biological and environmental hazard protection.



Radar wave fringe pattern on X24C-10D re-entry vehicle

Mach3: A Three-dimensional MHD Code for Parallel Computers

U. Shumlak
Phillips Laboratory, Kirtland AFB, NM

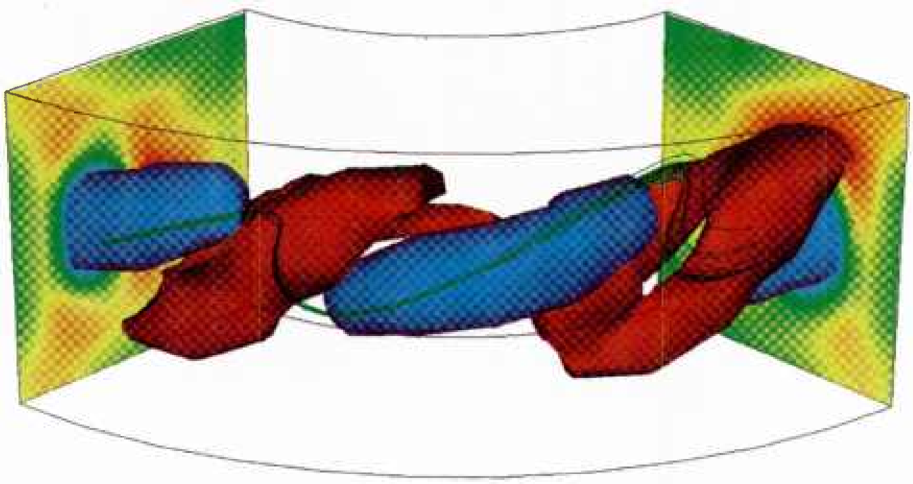
Computer Resource: IBM SP1 [MHPCC, Kihei, HI] and Cray Y-MP and C-90 [CEWES, Vicksburg, MS]

Research Objective: To develop Mach3, a three-dimensional magnetohydrodynamic (MHD) code for parallel computers and to apply this code to investigate space debris and nuclear weapons simulators.

Methodology: The equation set used in Mach3 is the time-dependent, nonlinear, single-fluid, two-temperature MHD plasma model. The equations are solved by using an equation-splitting technique to form constituent equations (diffusion, Lagrangian hydrodynamics, and advection). Diffusion is solved by using Brandt's full approximation storage multi-grid algorithm, the Lagrangian hydrodynamics are solved by using a Newton procedure, and the advection equation is solved explicitly with a Van Leer transport algorithm. The implicit schemes provide flexibility in examining the time scales of interest without the tight time step constraint that is present in explicit algorithms. The MHD equations are solved on a nonuniform, 3-D mesh. The mesh is composed of user-defined blocks that are connected to span the computational domain. Mach3 was written with its multi-block domain structure for the ultimate goal of porting the code to a massively parallel computer. All communication that occurs between blocks is performed by using pseudo message-passing routines, so Mach3 is already a "simulated-parallel" program. The computational domain will be distributed on the nodes of a parallel computer (one block per node), and the pseudo message-passing routines will be replaced with calls to a message-passing library.

Results: The serial version of Mach3 has recently matured beyond its developmental stage. The code has been applied to several applications. The most significant are magnetic diffusion in our liner implosion system and relaxation of nonaxisymmetric toroidal plasmas (see figure). The Mach3 code has given design guidance for the liner implosion system that is currently under study. The liner implosion system isotropically compresses plasmas to high pressures, which can then be used to generate hypervelocity projectiles for space debris simulation and to study catalyzed fission/fusion. A paper describing the details of this design guidance has been submitted to the *IEEE Journal Transactions on Plasma Sciences*. The code has also provided insight into the relaxation process of the toroidal plasmas that are being investigated. Toroidal plasmas are accelerated to high velocities and then stagnated to produce short pulses of X rays, which simulates a nuclear weapon detonation for studying weapons effects and nuclear fusion. When the code has been completely ported to a massively parallel computer, Mach3 will be used to simulate the entire process of X-ray production using toroidal plasmas.

Significance: The 2-D version of the code is currently being used by several universities and NASA and DOE laboratories to study the grand challenge problem of fusion power, electric space propulsion, and other plasma devices. When Mach3 reaches the stage of a production code, it will also be distributed as widely.



High (darker surfaces) and low (lighter surfaces) density isosurfaces and kinked magnetic field lines resulting from a nonaxisymmetric density initialization

Climate/Weather/ Ocean Modeling

Climate, Weather, and Ocean is concerned with the accurate numerical simulation and forecast of oceanic and atmospheric variability for both scientific and operational use. CWO is used within DoD for safety of flight, mission planning, optimal aircraft and ship routing, anti-submarine warfare, and weapon system design.

These CWO success stories were chosen to illustrate both this wide range of applications and the grand challenge nature of basic research. In addition, contributions were selected from both major Service laboratories and DoD sponsored (ARO, AFOSR, ONR, and DNA) academic research. The success story by Jacobs represents a major breakthrough; it was featured on the cover of the journal Nature *and was the subject of an article in the* New York Times. *The success story of Preller et el. was a part of a congressionally mandated effort to investigate the potential dispersal of Soviet Union radioactive contaminants located in the Kara Sea. The application of the Krishnamurti model to the understanding of Hurricane Andrew has clear societal benefits.*

Dr. Joseph W. McCaffrey, Jr.
Naval Research Laboratory
CTA Leader for CWO

Long Time Period Adjustment of the Large Scale Ocean Climate

Gregg Jacobs

Naval Research Laboratory, Stennis Space Center, MS

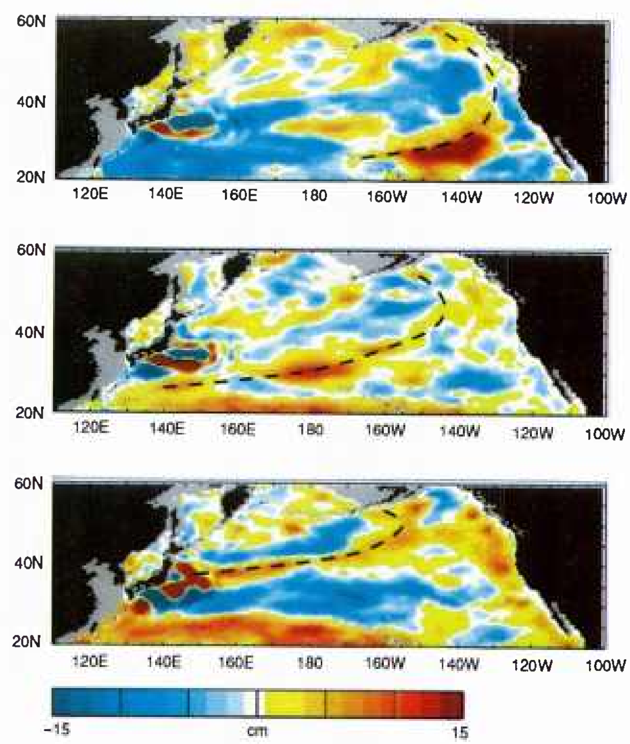
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS] and Y-MP/8/8/128 [NAVO, Stennis Space Center, MS]

Research Objective: To understand the decadal scale oceanic variability

Methodology: Using a combination of satellite altimeter measurements of sea surface height (SSH), satellite infrared measurements of sea surface temperature (SST), and a numerical global ocean model, NRL investigated the long-term impact of the 1982-83 El Niño. While variations in oceanic forcing, such as winds or thermal radiation, occur at relatively short time scales on the order of weeks to a year, the ocean circulation and climate driven by these changes in forcing can take years to decades to respond at the large scale. The long time period response of the ocean is provided through Rossby waves.

Results: Research work conducted at NRL was the first to reveal Rossby waves produced by extreme climatic events such as the 1982-83 El Niño. The 1982-83 El Niño Rossby wave was initiated at the American coasts and had reached Japan by 1992. Upon reaching Japan, the wave interacted with the Kuroshio Extension to produce SST anomalies over 1°C extending across the Pacific Ocean [G.A. Jacobs, H.E. Hurlburt, J.C. Kindel, E.J. Metzger, W.J. Teague, and A.J. Wallcraft, "Decadal-Scale Trans-Pacific Propagation and Warning Effects of an El Niño Anomaly," *Nature*, **370**, 360-363 (Aug. 1994)].

Significance: SST anomalies, such as those observed in this study, have been shown to have significant impact on weather patterns throughout the world. (Indeed, the weather in Alaska was unusually warm during the summer of 1993.) These results indicate that oceanic climate on the large scale changes very slowly. However, model results indicate that the climate variations produced by these waves are very predictable. The remarkable sequence of events uncovered by this investigation indicates the surprising long-term oceanographic effects of the major 1982-83 El Niño. The methods employed in this investigation—numerical modeling and satellite oceanography—aptly illustrate the utility of the critical components of a global ocean observing and prediction system. Global ocean monitoring and prediction systems have applications ranging from military operational support to studies of global environmental change, including (a) military operations, such as safety of flight, ship and aircraft routing, search and rescue, ASW, and coastal and mine warfare; (b) commercial applications, such as ship-routing and fisheries forecasts; and (c) global environmental monitoring and prediction, such as pollutant-spill risks, El Niño forecasting, and ocean observing system simulations.



Predicted 1-yr average SSH deviations from an 11-yr mean: (top) 1-yr average for the period Mar. 1984 to Feb. 1985; (center) 1-yr average for the period May 1987 to Apr. 1988; (bottom) 1-yr average for the period Apr. 1992 to Mar. 1993. Solid lines indicate the Rossby wave signal from the 1982-83 El Niño.

High-Resolution Atmospheric Forecast Model with Physical Initialization

T.N. Krishnamurti, Kevin Ingles, Darlene Oosterhof, and Gregory Rohaly

Florida State University, Tallahassee, FL

Office of Naval Research, Arlington, VA

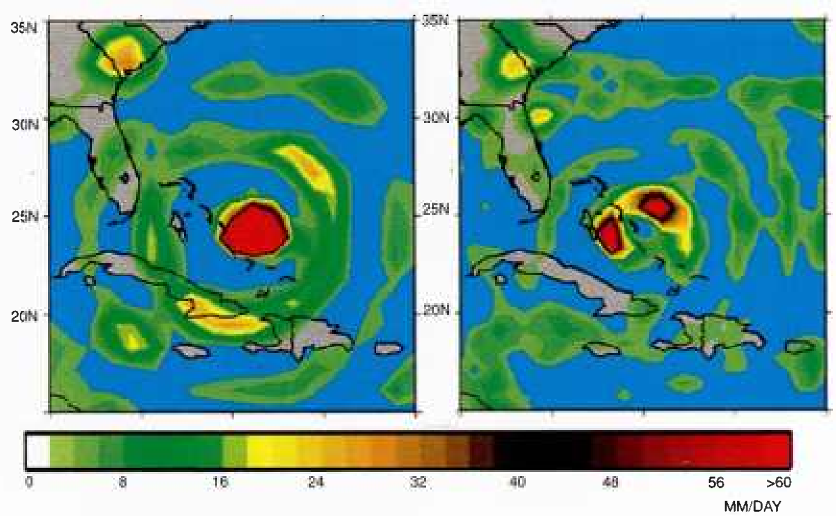
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: To improve atmospheric model forecasts for potentially severe tropical disturbances (development, intensity, and track) and mesoscale and submesoscale features related to sea breeze, terrain interactions, diurnal effects, and surface fluxes.

Methodology: The FSU global spectral model at T213 horizontal resolution (720 x 320 gaussian grid, approximately 0.5°) and 14 atmospheric levels is used for mesoscale study of tropical disturbances. The addition of physical initialization imports satellite data along with the initial World Weather Watch data. This technique enhances the definition of surface fluxes of water vapor and sensible heat in addition to precipitation and clouds.

Results: Our study, which includes physical initialization with the use of a very high resolution global model, indicates that this technique is a useful procedure for the nowcasting of rainfall. Correlation between model based initialized rain and satellite-raingauge based rain over the entire tropics (for 6-hour averages and averaged over transform grid squares) is of the order of 0.85. This compares with corresponding numbers of around 0.3 for models that do not include physical initialization. The 1-day tropical rainfall skill is also very high for the physically initialized experiments; the correlation is of the order of 0.55. The lifetime of mesoconvective systems is typically of the order of 1 day. Most of the tropical rainfall is associated with these systems; hence the skill beyond 1 day degrades somewhat. However, the model does seem to capture the 1-day passage of mesoconvective systems; these systems exhibit a robust vertical structure of divergence, heating, and vertical motion. The organization of mesoconvective systems (sweeping by large scale circulations and the coalescence of mesoscale elements) appears to play an important role in the formation of tropical storms. The vorticity of these mesoscale elements, however, does not exhibit any interesting organization as the storms form. The model at the resolution T213 discerns the eye and the outer rain bands of Hurricane Andrew of 1992, which appears similar to the radar imagery; however, the scales are roughly three times larger. Further enhancement of resolution is needed to model realistic storms. Our study demonstrates that mesoconvective elements are in fact simulated by very high resolution global models. A research paper entitled "Meso-scale Structure Implied by Physical Initialization," which describes this study, was submitted to *Monthly Weather Review* in July 1994. This paper acknowledges the use of HPC resources.

Significance: Improvements listed under research objective are necessary for missile launch and ship support.



Mesocale rainfall bands for Hurricane Andrew (24 Aug 1992) for model resolutions T106 (left) and T170 (right).

Atmosphere/Ocean-Wave Model Simulations of Cyclogenesis in the Coastal Zone

James D. Doyle
Naval Research Laboratory, Monterey, CA

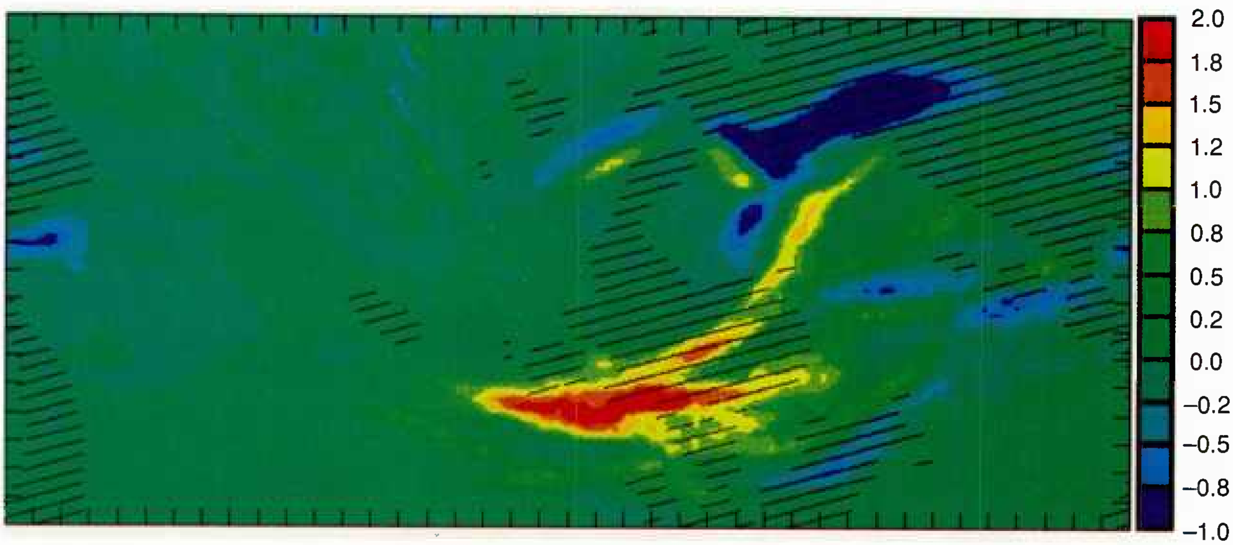
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: Regional meteorological forecasts of cyclones in the coastal zone are often inadequate, in part, because of a lack of understanding of the air-sea interaction processes. The specific objective is to investigate the impact of the roughness effects of ocean waves on the coastal atmospheric environment during extratropical cyclogenesis.

Methodology: The Navy's Coupled Ocean-Atmosphere Mesoscale Prediction System (COAMPS) is coupled in a mutually interactive manner to the wave model (WAM); this marks the first time that such a modeling system has been used anywhere. The coupled model is fully vectorized and multi-tasked to take full advantage of the CEWES supercomputers.

Results: Young or growing ocean waves modulate the heat, moisture, and momentum transport between the atmosphere and ocean. As a result, regional-scale structures such as rainbands and fronts associated with the cyclone are perturbed (see figure). The cyclone intensity and energy balance are significantly impacted as the result of ocean-wave enhanced roughness.

Significance: Extreme weather conditions associated with extratropical cyclones can have an adverse impact on U.S. Navy operations such as navigation conditions, radar propagation, communications, search and rescue operations, coastal warfare, and weapons systems. Potential commercial applications include ship routing and coastal and marine weather forecasting. Without adequate warning, coastal cyclones can cause widespread property damage and loss of life. This study represents a first step in unraveling the intricacies of the coupled ocean-atmosphere response in the coastal zone on regional and small scales.



Simulated difference in rainfall rate [cm (12 h^{-1})] resulting from enhancement of the surface roughness associated with ocean waves. Positive (negative) values correspond to an increase (decrease) in rainfall due to ocean waves. The hatched regions represent areas of young ocean waves. The region of the simulation domain shown is 1800 x 4000 km.

Aircraft Icing

George D. Modica and Scot T. Heckman
Phillips Laboratory, Hanscom AFB, MA

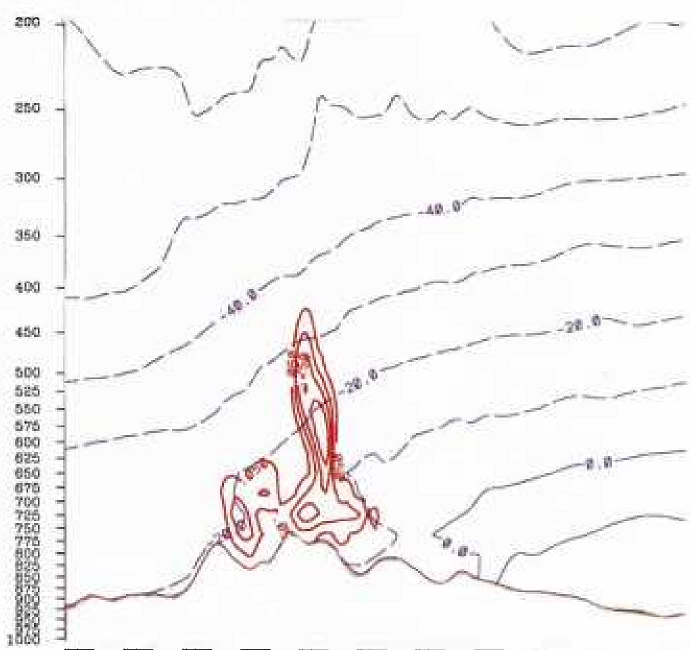
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To determine whether a regional mesoscale model with a modified microphysics parameterization can provide deterministic forecasts of aircraft icing conditions (supercooled liquid water (SLW)) in the 6- to 36-hour time frame.

Methodology: A regional numerical weather prediction (NWP) model was modified to permit the existence of both liquid and ice hydrometeors within the same grid volume. The algorithm was built around the National Center for Atmospheric Research/Pennsylvania State University mesoscale model (MM4). This is a Eulerian gridpoint model that uses finite-difference approximations to the continuous system of equations and has second-order accuracy. The model uses the explicit centered-in-time centered-in-space time integration. The original model incorporated a bulk microphysics type of precipitation parameterization for either liquid or frozen hydrometeors within a particular grid volume, but not both. The modified model includes an efficient ice-water saturation adjustment and a simple procedure to create or remove cloud water or ice, both of which were taken from earlier cloud-scale modeling studies. The model was used to simulate an orographically forced icing event in which an SLW cloud formed and was sustained for more than 48 hours over the northern front range and plains of eastern Colorado. This event was responsible for a crash of a civilian aircraft and the death of its pilot.

Results: Output from a 24-hour forecast from the model was compared to observations taken during the Winter Icing and Storms Project-1990 (WISP-90). The model produced a thin (1 to 2 km deep) SLW cloud that was in good agreement with observations in terms of initiation, duration, liquid water content, and location. The model forecast also revealed mechanisms that could be responsible for generating SLW at higher levels in the troposphere [G.D. Modica and S.T. Heckman, "An Application of an Explicit Microphysics Mesoscale Model to a Regional Icing Event," *Monthly Weather Review* **33**, 63-64 (1994)].

Significance: This line of research has important implications for combat weather support where aircraft operations are required. Improved predictions of clouds and associated aviation impact variables (e.g., precipitation, icing, downbursts) are relevant to the civilian aviation community and other more general interests that are affected by weather.



Vertical cross section of 6-hour forecast cloud liquid water (g kg^{-1}, solid red) and temperature (°C, dashed blue), between north-central Montana (left) and central Texas (right)

Diagnosing Clouds from Weather Prediction Model Forecasts

D.C. Norquist, H.S. Muench, D.C. Hahn, and D.L. Aiken
Phillips Laboratory, Hanscom AFB, MA

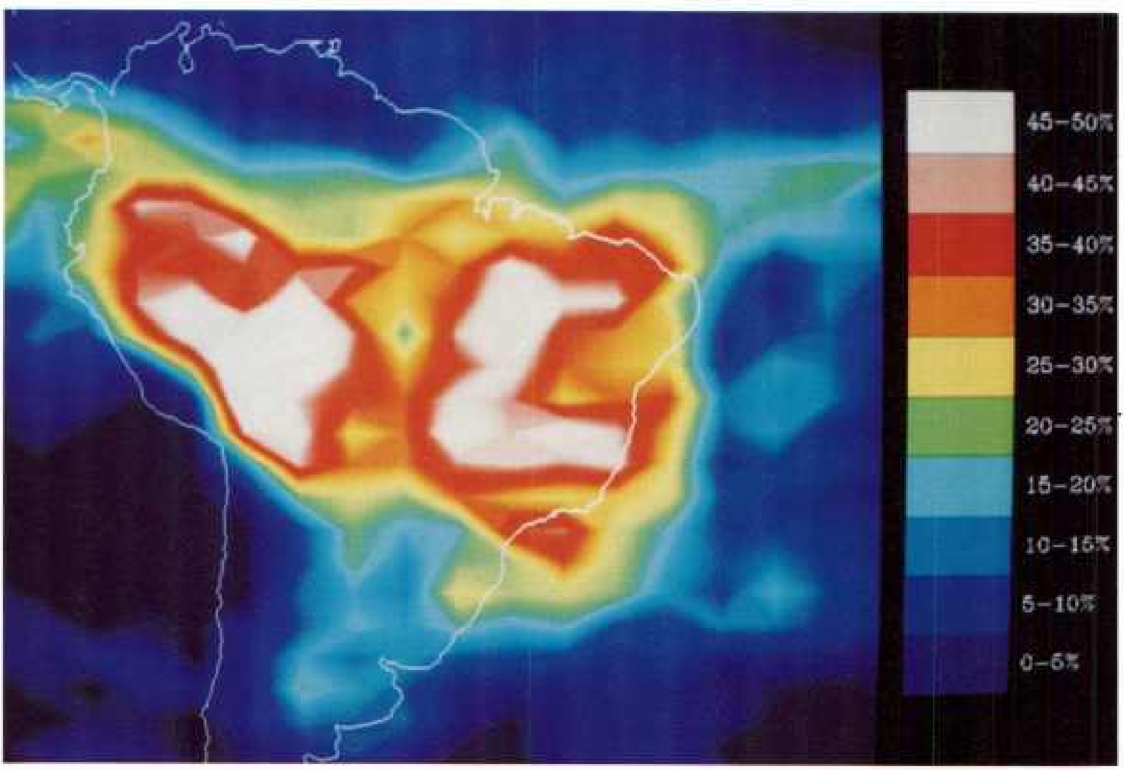
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To determine the extent to which noncloud meteorological predicted variables from a global numerical weather prediction model forecast can be used to diagnose cloudiness at forecast times.

Methodology: We executed twice-daily weather forecasts out to 48 hours of forecast time using the Phillips Laboratory Global Spectral Model for 1 to 24 January and July 1991. Each forecast required about 2.5 hours CPU time on the Cray C-90 run in multi-tasking mode. We transformed USAF RTNEPH cloud analyses onto a common grid (125-km spacing in the horizontal; low, middle, and high cloud decks in the vertical) to establish a one-to-one spatial correspondence with the weather forecast variables. A subset of meteorological variables available from the forecast fields was used as a predictor; transformed RTNEPH cloud amounts were used as predictands in 10-day development periods to develop statistical predictand-predictor relationships using multiple linear regression. These relationships were applied to weather forecasts initialized on day 11 to diagnose cloud amounts at forecast times of 12 and 48 hours.

Results: Both 12- and 48-hour cloud forecasts derived by using the multivariate diagnostic method were superior to univariate methods that used only relative humidity as a predictor. The potential of using noncloud forecasts to deduce cloud forecasts was demonstrated.

Significance: In warfighting, knowledge of locations and amounts of near-future cloud cover is crucial in USAF mission planning. Civilian uses of cloud diagnostic techniques include cloudiness specification in general circulation models used in climate change research.



Average day-night difference in model-deduced high cloud cover (%) during a season of intense convection over the Amazon basin

Effects of River Outflow on Sea Ice in the Kara and Neighboring Arctic Seas

Ruth H. Preller and Richard Allard
Naval Research Laboratory, Stennis Space Center, MS

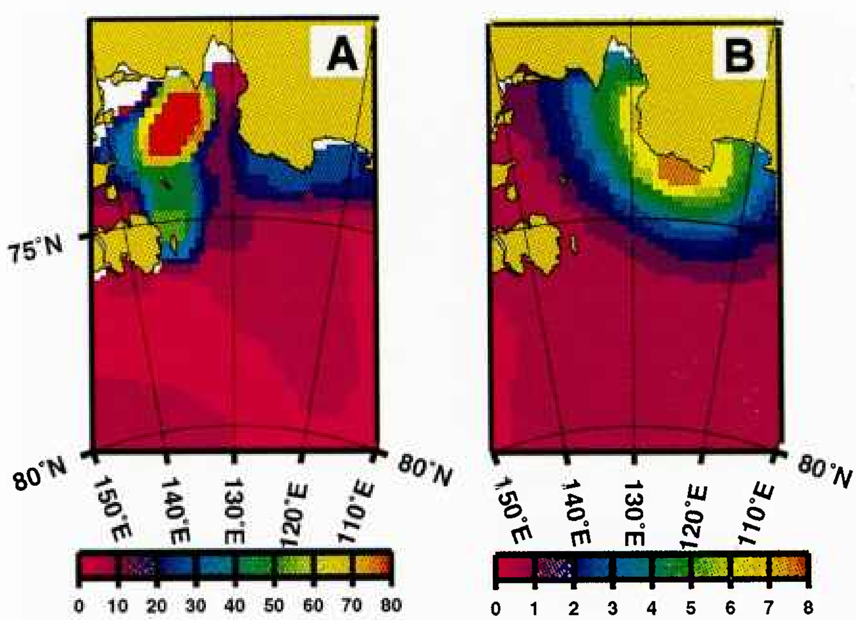
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To determine the effects of a monthly varying salinity and temperature flux, due to river outflow, on the growth/decay and the circulation of sea ice. A 50-year Russian data set of monthly river discharge enabled us to look at this effect in a more realistic manner than it had been done before.

Methodology: The effect of freshwater river discharge on the Arctic circulation and its ensuing effect on the growth and melt of sea ice was examined using a coupled ice-ocean model. A freshwater salinity flux was specified at the gridpoints surrounding nine major rivers discharging into the Arctic shelf region. The temperature of the discharged water was also specified. The model had a 25 km horizontal grid spacing, representing 129,600 grid points with 15 vertical levels in the ocean model. This model, requiring 32M words of memory, required the resources of a Cray C-90. The model was driven with monthly mean Navy atmospheric forcing and a recently obtained Russian data set of river outflow.

Results: The inclusion of freshwater discharge into the Arctic via rivers greatly affected the ocean circulation near the river mouths. The ocean currents tended to first flow northward and then turned to the right of the less dense surface waters. River discharge is at its peak in June, where surface currents near the Lena River were near 6 cm/s (compared to 1 cm/s without rivers). The addition of warmer river water caused ice to form more quickly than in the no-river case. The ice thickness difference (see below) between the cases with and without rivers was often as large as 1 m after a year of model simulation.

Significance: River outflow causes local changes in ocean circulation, ice drift, and the growth and decay of sea ice near river mouths. Over time, changes in atmospheric forcing (winds, heating, and cooling) can cause these local changes to impact larger regions of naval interest. Therefore river outflow must be properly included in the prediction of ice and ocean conditions to improve navigation in ice covered seas.



(A) Ice thickness difference (cm) between the no-river and the 50-yr mean discharge case in the Laptev Sea on 31 August 1986; (B) same as for (A) but for salinity difference (PPT)

Spectral Wave Forecast System

R. E. Jensen and W. R. Curtis
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

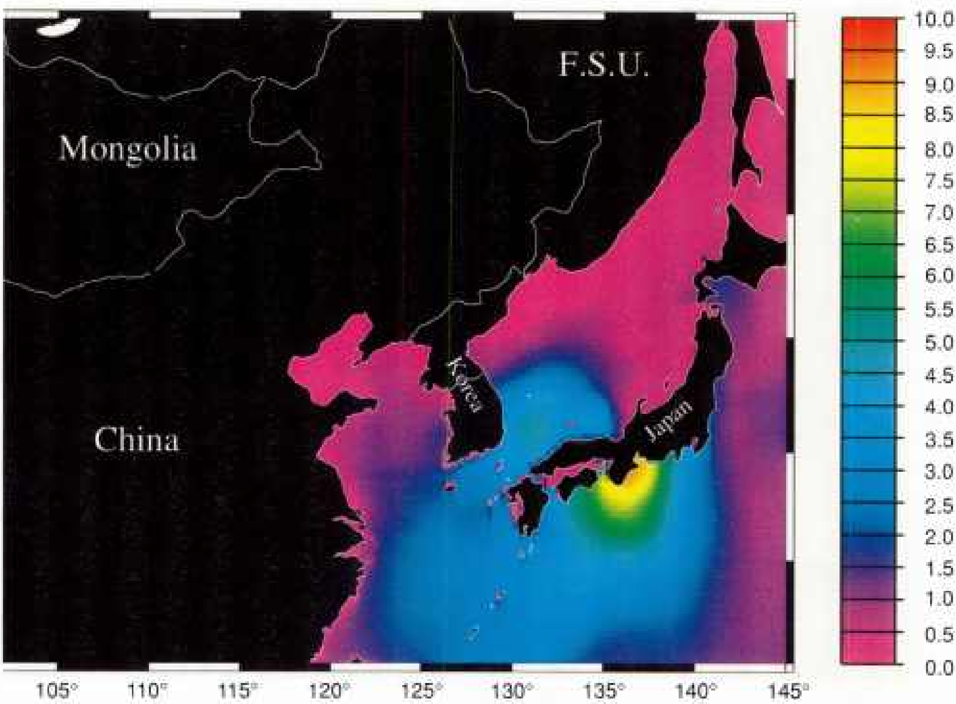
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To develop, test, and implement a state-of-the-art, third generation discrete spectral wave model for the simulation of accurate, worldwide wave information in either a forecast or hindcast mode.

Methodology: The USAE Coastal Flooding and Storm Protection Program cooperated in a research initiative formed by the Wave Modelers (WAM) Group, a consortium of mainly European scientists developing a new generation wave model technology. This model, called 3GWAM, solves the energy balance equation for the temporal and spatial changes in directional wave spectra. Unlike its predecessors, 3GWAM avoids a priori assumptions governing the spectral shape by explicitly solving the source/sink mechanisms (atmospheric input, nonlinear wave-wave interaction, high-frequency dissipation, and wavebottom effects) discretely rather than in a parametric form. The computational time for these calculations is significant. However, under complex meteorological scenarios (rapid wind shifts, hurricanes, frontal passages), 3GWAM results are far more accurate than results from contemporary second- and first-generation models. 3GWAM has undergone massive testing and validation, and code efficiency is optimized by use of vector processing—300 to 400 Mflops on a single CPU.

Results: The Naval Oceanographic Office (Stennis Space Center, MS) in collaboration with CEWES, is now implementing 3GWAM in a forecast mode for eight areas of responsibility (AOR) worldwide. Beta testing of 3GWAM and development/application of the wave forecasting system were conducted at CEWES. To accompany these twice-a-day forecasts, rapid response wave forecasting systems have been built, and the wave model results have been used in direct support of ongoing military exercises.

Significance: Because of the need for a highly mobile military, accurate forecast wave estimates in operational areas are critical for the planning and execution of logistics over the shore. Using 3GWAM for these purposes has proven to be highly successful.



Wave height color contours (meters) for Typhoon Yancy (September 1993)

Eddy-resolving Global Ocean Modeling and Prediction

Harley E. Hurlburt and Alan J. Wallcraft
Naval Research Laboratory, Stennis Space Center, MS

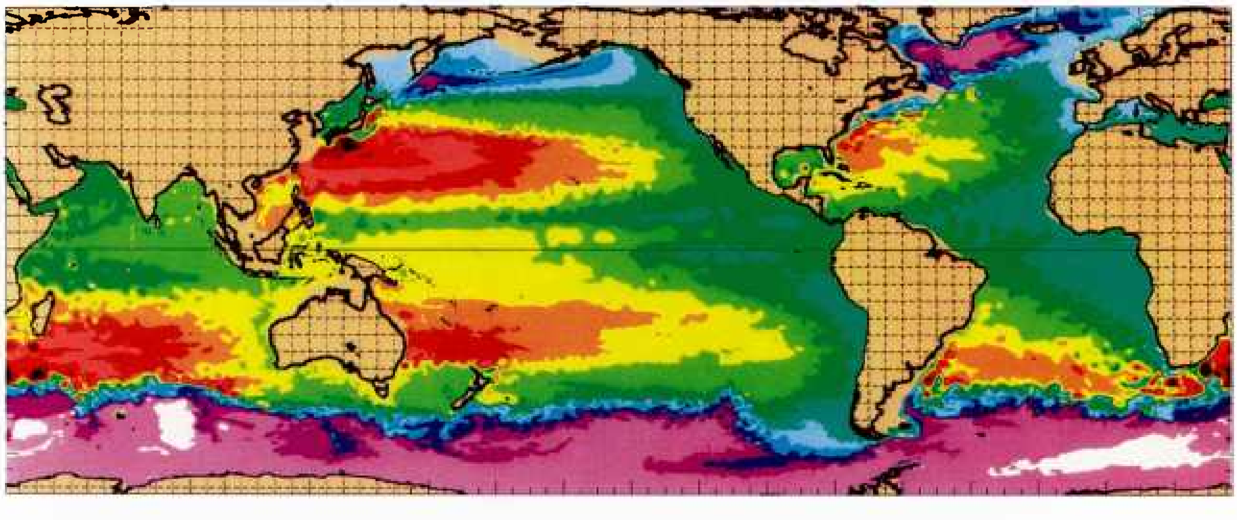
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS] and TMC CM-5E [NRL, Washington, DC]

Research Objective: To develop an eddy-resolving global- and basin-scale ocean monitoring and prediction system. This includes understanding ocean dynamics, model validation, naval and global change applications, ocean predictability, and observing system simulation.

Methodology: The NRL layered ocean model is typically ten to hundreds of times more efficient than other global ocean models. This is primarily because Lagrangian layers are used in the vertical and a semi-implicit time scheme makes the time step independent of all gravity waves (but requires the solution of Helmholtz's equations). The Helmholtz's solver used is very efficient, but has large memory requirements. The 1/8 degree global model requires about a gigaword of memory.

Results: The world's first eddy-resolving, 1/8 degree, global ocean model was demonstrated on the CEWES C-90, but it is too large to run in the CEWES normal job stream. It is now running on the NRL CM-5E.

Significance: Eddy-resolving global ocean modeling is a grand challenge problem. By careful choice of algorithms, we have been able to run such a model on existing supercomputers, which are orders of magnitude away from Tflops performance. Eddy-resolving models are an important milestone on the road to global monitoring and prediction systems. Applications include military operations such as search and rescue, antisubmarine warfare, coastal and mine warfare, and commercial applications such as ship routing, fisheries forecasts, and global environmental monitoring and prediction, e.g., pollutant spill risks, El Niño forecasting, global change studies, and ocean observing system simulation.



Sea surface height snapshot from a 1/8 degree global ocean model. The model was spun up from rest, driven by monthly climatological winds, at lower resolution for 224 years, and has run 3 years at 1/8 degree. Contour interval is 12.5 cm.

Development of Continental-Scale Databases

N.W. Scheffner and H.L. Butler
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

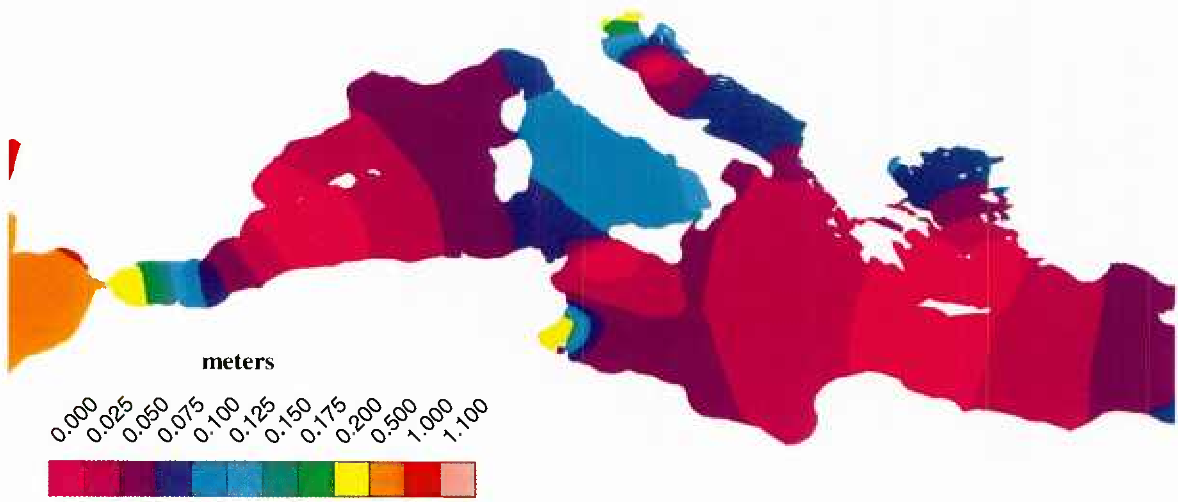
Computer Resource: Cray C-90 [CEWES, Vicksburg, MS]

Research Objective: To develop tidal and frequency-indexed storm surge databases on a continental scale.

Methodology: The USAE Dredging Research Program has developed a large-domain, advanced hydrodynamic circulation model (ADCIRC) for both tidal circulation and storm surge propagation. The model is based on a finite-element numerical solution of the generalized wave-continuity equation (GWCE). GWCE-based solutions to the shallow-water equations allow for extremely flexible spatial discretizations. A highly efficient code is accomplished by (a) decoupling of the time and space discrete form of the GWCE and momentum equations, (b) using time-independent and/or tridiagonal system matrices, (c) eliminating spatial integration procedures during time stepping, and (d) vectorizing all major computer code loops.

Results: This technology was used to simulate tidal and storm surge propagation over continental-scale computational domains, such as the single 30,000-node east coast, Gulf of Mexico, and Caribbean Sea grid. These simulations have resulted in a user accessible database of tidal constituents over the entire computational domain and storm elevation and current time series at selected nearshore locations along the coasts. Technology transfer to military needs has been successfully accomplished as exemplified by use of ADCIRC to (a) simulate and supply circulation information for logistics over-the-shore operations in the Persian Gulf and (b) develop tidal and current constituent databases for several Naval Oceanographic Office areas of responsibility (AOR) such as the Mediterranean Sea.

Significance: The GWCE-based model is a breakthrough technology for solving large-scale hydrodynamic modeling problems. For civil works projects, the tidal and storm surge databases are critical for developing accurate design criteria and data for risk assessment. In the military arena, forecast capability for AOR coastal hydrodynamics is essential.



M_2 tidal amplitude in the Mediterranean Sea using a 12,600-node GWCE model grid

Effects of the Flow Through the Maritime Region on the Upper Tropical Pacific and Indian Oceans

James J. O'Brien
Florida State University, Tallahassee, FL
John C. Kindle
Naval Research Laboratory, Stennis Space Center, MS
Mark A. Verschell
Florida State University, Tallahassee, FL
Office of Naval Research, Arlington, VA

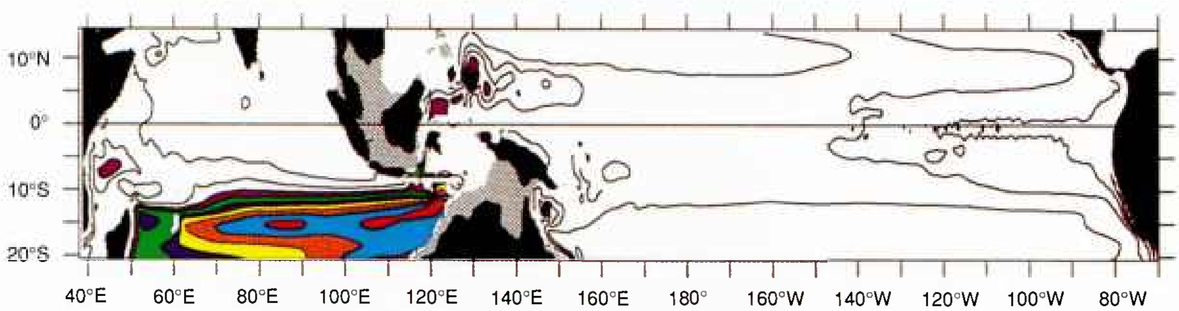
Computer Resource: Cray Y-MP [NRL, Stennis Space Center, MS]

Research Objective: To investigate the dynamics and influence of the Indonesian throughflow region on the upper Pacific and Indian oceans (PACIO) by using a reduced gravity global ocean model.

Methodology: A global reduced gravity ocean model with 0.5° latitude, 0.7° longitude horizontal resolution was implemented for the global oceans. The model was forced with realistic winds, i.e. a 10-year (1980-1989) monthly climatology of surface winds from European Centre for Medium-range Weather Forecasting (ECMWF). Two independent experiment sets were identical except that different coastline geometries were used to understand the effects of PACIO throughflow. The model geometries differed only in whether PACIO throughflow was permitted.

Results: The Open experiment yielded a mean westward transport through the PACIO region of 7.5 ± 4.75 x 10^6 m^3s^{-1}. Episodes of large eastward transport were determined to be linked to passage of interannual Rossby wave energy from the Pacific to the Indian Ocean during the northern winter following an El Niño/Southern Oscillation (ENSO) warm event. There appears to be no appreciable effect of PACIO transport on interannual variability in the eastern tropical Pacific. The average upper layer thickness of the Indian Ocean was much deeper and more variable because of the influence of PACIO transport, while the effect in the Pacific Ocean was much smaller. Differences between the Open and Closed cases showed areas of low frequency (greater than one-half year) variability over most of the southern Indian Ocean, the western boundary of the Indian Ocean, the region of the Mindanao eddy, and the eastern Pacific equatorial waveguide. Areas of significant high-frequency variability were the East African coastal current near the generation region of the Great Whirl, the Mindanao eddy region, the Coral Sea basin, and in the eastern equatorial Pacific waveguide.

Significance: An understanding influence of the Indonesian throughflow on the dynamics of Pacific and Indian Oceans will have both societal (El Niño forecast) and military (mission planning) benefits.



Total RMS difference (open-closed) in upper layer thickness in meters over a 10-year period for the tropical Pacific and Indian Oceans.

Signal/Image Processing

Embedded Signal and Image Processing applications convert raw sensor information into higher level information through processes such as automatic target detection, recognition, and tracking. The rapid advance of HPC technology allows the hard-wired, one-of-a-kind systems used today to be replaced with scalable and programmable open systems, which increases competition and greatly reduces cost.

The following success stories show HPC technology meeting the real-time throughput requirements posed by two radar and two sonar applications. In all these cases, HPC technology is not just proving feasibility in the laboratory, but moving to the field with low-cost embedded computing solutions.

Dr. Richard W. Linderman
Rome Laboratory
CTA Leader for SIP

Acoustic Signal Processing

W. Anderson, H. Shyu, and W. Smith
Naval Research Laboratory, Washington, DC

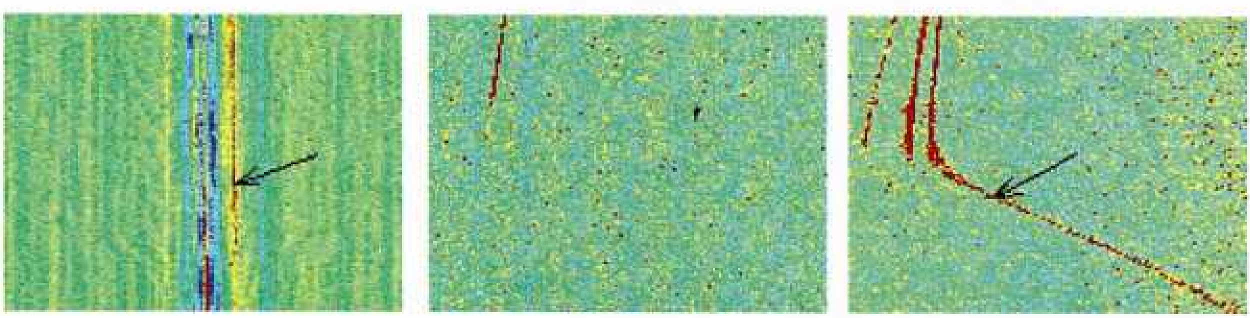
Computer Resource: TMC CM-5 [NRL, Washington, DC]

Research Objective: Antisubmarine warfare operations involve quiet targets in littoral and congested environments and require advanced techniques for improved detection, rapid localization, and high-resolution tracking. New array configurations and difficult environments require computationally intensive algorithms and high-performance systems to process high-dimensionality data. The full spectrum of sources and sensor configurations must be utilized. The object of this research is to assess the exploitability of broadband energy sources for this purpose.

Methodology: Processing strategies include intra- and intersensor correlation of broadband energy over extended time, frequency, and space with compensation of Doppler and array beam parallax effects. The system processing flow involves a mix of filtering, transformation, beamforming, correlation, integration and other functions. Data arrays and processes map well to the Connection Machine (CM) architecture. The size of the CM main memory enables large multi-dimensional data (i.e., spatial beam, spectra, Doppler bin) transformation and aggregation operations to be processed in situ, avoiding unacceptable overhead caused by secondary storage thrashing. Signal correlation results are evaluated over various ranges of integration time, frequency bands, time delay, and Doppler to assess target parameters, propagation, and environmental background effects.

Results: Broadband correlation has been tested on distributed array data. Successful target correlation has been obtained over baselines of up to 30 km, time-bandwidth products greater than 104, and relative Doppler up to 18 kt. Signal-to-noise ratio improvement of more than 15 dB was observed on long correlation sample lengths (2048K), provided Doppler compensation was applied. The figure shows broadband correlograms produced from local sensor nodes (left) separated by a few yards with that from nodes separated by 15 km (right). A correlogram horizontal axis measures time delay difference of arrival or source bearing, and the vertical axis measures elapsed time. On the left, the target trace (arrow) is seen along with other ship traces; accurate measurement of time delay or bearing history is limited by the small intersensor aperture. On the right, the bearing scale is significantly extended and the target trace more highly resolved, presenting a more informative picture regarding target location and motion. The center correlogram shows the results of wide aperture correlation without Doppler correction and long correlation window; the trace is lost in the background noise for most of the run.

Significance: These techniques can be applied to detection and localization of both underwater and surface vessels for military and commercial traffic surveillance and interdiction. Additionally, this experience with the CM demonstrates and validates the value of parallel high-performance computer technology for real signal processing application systems in the Navy. Specially designed military signal processors are no longer a necessity for most system applications.



Broadband correlograms

Hybrid Digital/Optical Processor

R. A. Dukelow and R. M. Hidinger
Naval Command, Control and Ocean Surveillance Center, San Diego, CA

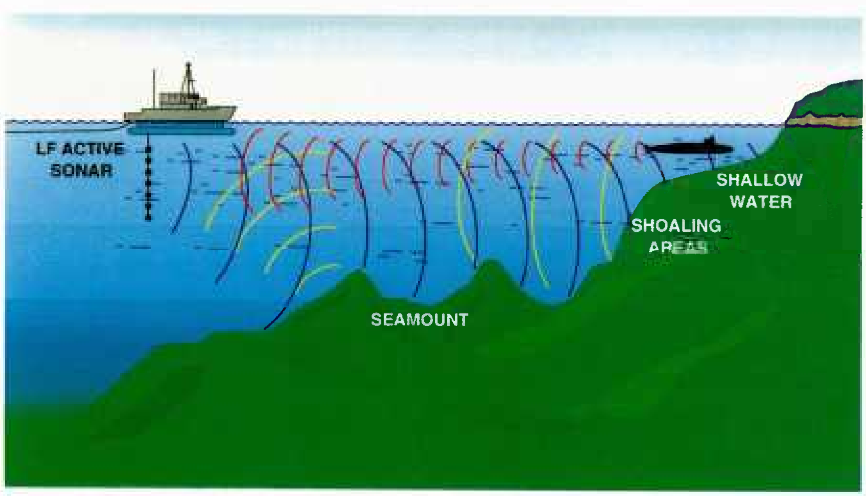
Computer Resource: Intel Paragon XP/S-25 [NRaD, San Diego, CA]

Research Objective: To demonstrate the feasibility of using embedded scalable high-performance digital and optical processing to solve the problem of submarine detection and classification in shallow water.

Methodology: The HyDOP objective requires applying computationally intensive algorithms that cannot be implemented in real time by using conventional processors. The sonar system chosen for the initial HyDOP demonstration is the low-frequency active component of the Surveillance Towed Array Sensor System (SURTASS/LFA). A high-speed optical correlator being developed by the Naval Research Laboratory will act as a coprocessor to the Paragon. Other specialized interfaces to the Paragon are also being developed for possible at-sea demonstrations. This project has been made possible only through the cooperative investment by the Office of Naval Research (ONR-321) and the DoD HPC Modernization Program, which established the NRaD Shared Resource Center with a special emphasis on supporting classified, real-time, embedded processing research projects such as HyDOP.

Results: Tools and techniques have been developed for using scalable processors in real-time, embedded systems. A Scalable Programming Environment (SPE) has been designed to support development of data-flow-oriented programs typical of this type of application. A prototype SPE has been used to implement a run-time scalable baseline processing string. This processing string has demonstrated nearly linear performance scaling—from about 2x real time using 12 processors to about 7x real time using 38 processors. The processing capabilities demonstrated to date show that scalable processing technology can be successfully applied to real-time, embedded sensor applications. Full implementation of the SPE and the HyDOP advanced algorithms are continuing.

Significance: The shallow-water acoustics problem has become increasingly important because of the heightened threat of regional conflicts, where the Navy is likely to encounter slow, diesel submarines close to shore. Unfortunately, the shallow-water, slow submarine is significantly more difficult to detect and classify acoustically than the traditional deep-water, fast nuclear threat as a result of the complex propagation, high clutter, and low target Doppler. Achievement of effective sonar performance requires new processing algorithms that cannot be implemented on current naval platforms because of the high processing requirements. The experience gained should be applicable to other nonacoustic sensor systems such as radar and optics.



SURTASS/LFA sonar system operating in shallow water

Embedded Space-Time Adaptive Processing for AEW Radars

R. Kohler, R. Linderman, and D. Rabideau
Air Force Rome Laboratory, Rome, NY

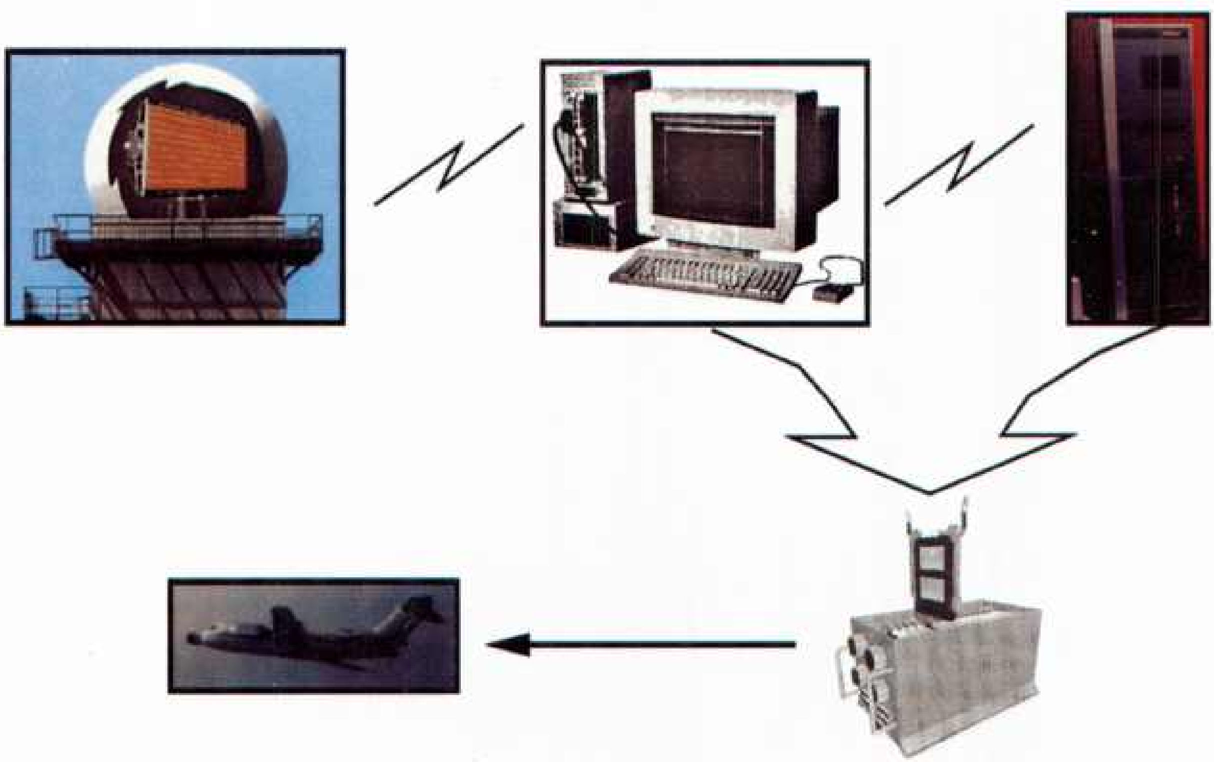
Computer Resource: Intel iPSC/860 [Rome Lab, Rome, NY]

Research Objective: To improve clutter and jamming suppression on airborne early warning radar (AEW) systems by implementing real-time space-time adaptive processing on HPC architectures.

Methodology: Real-time inputs from a C-Band phased array radar were fed into an Intel iPSC/860 and Sun workstation for real-time processing and display. Adaptive beamforming weights were calculated and applied to the received data to implement a post-Doppler version of space-time adaptive processing (STAP).

Results: The iPSC/860 implemented the matrix factorization and weight calculation operations in a real-time application environment. STAP canceled clutter and jamming in the phased array radar returns permitting greater radar sensitivity that led to the detection of smaller targets. Results were updated in real time on the Sun workstation under an X Windows graphical environment.

Significance: Improving the performance of AEW radars against advanced threats requires more complicated and computationally intensive signal processing algorithms, such as STAP, to be performed in real time. The complexity of the matrix manipulations involved in STAP processing grows as the cube of the number of radar channels and quickly becomes a 50 to 500 Gflop challenge to solve within the size, weight, and power constraints imposed on an embedded system. This demonstration is a significant step in showing that HPC technology can meet these requirements with scalable solutions. Ongoing work is pursuing the next step of flying a version of the Intel Paragon HPC to perform STAP calculations for an airborne phased array radar.



Ground-based demonstration leads to embedded airborne demonstration

Scalable IFSAR DTE Processing

Chris Yerkes, Eric Webster, and Pieter Darnaud
Naval Command, Control and Ocean Surveillance Center, San Diego, CA

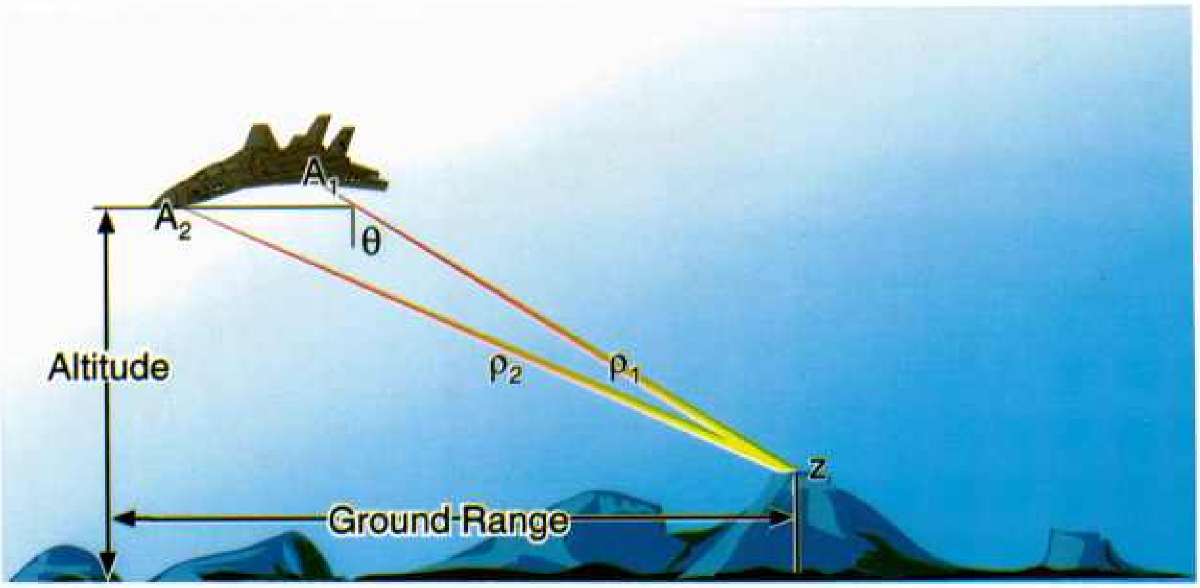
Computer Resource: Intel Paragon XP/S-25 [NRaD, San Diego, CA]

Research Objective: Recent advances in interferometric synthetic aperture radar (IFSAR) imaging technology have made timely production of low-cost, high-resolution digital terrain elevation (DTE) maps feasible. In the past, the computational complexity of SAR processing has dictated the design and use of special-purpose hardware. Such designs have been very costly and have had short life cycles. The objective of the Scalable IFSAR DTE Processing project is to demonstrate that current generation massively parallel processors (MPPs) can perform scalable IFSAR DTE processing in a production mode.

Methodology: The Intel Paragon computer was used because it represents a state-of-the-art MPP machine, and access to a Paragon system was readily available to the authors. The SAR image formation portion of the problem was implemented by using the single-program, multiple-data (SPMD) model. The current DTE algorithm is inherently sequential and was implemented as a three-stage pipeline. The SAR image formation code is efficiently scalable, up to a limit that is dependent on problem size. That is, as the problem size is increased, a larger machine can be used without loss of efficiency. At this point, the DTE code is not scalable.

Results: To date, two image-formation algorithms (ω-k and range-Doppler) as well as the IFSAR DTE algorithm have been successfully implemented on the Intel Paragon, and preliminary performance results have been obtained.

Significance: Implementation of this algorithm on a general-purpose MPP indicates that real-time SAR processing is possible without the need for special-purpose hardware. The results of the IFSAR DTE algorithm can be used for quick production of high-quality digital terrain elevation maps for commercial (nonmilitary) use or as part of an automatic target recognition system for military use.



IFSAR geometry. $A_{1,2}$ - antenna positions; z - ground height; $\rho_{1,2}$ - ranges; θ - look angle

Forces Modeling and Simulation/C^4I

Forces Modeling and Simulation/Command, Control, Communications, and Computers focuses on research that uses HPC to develop and deploy military systems. This type of computing is highly computer, data, and input/output intensive and normally operates in an interactive mode. Increased capabilities for handling these types of applications will result in additional success stories in the future. This year's success story addresses the generation of high-resolution terrain representations for use in combat simulation and synthetic environments.

Mr. Robert A. Wasilausky
NCCOSC Research and Development Division
CTA Leader for FMS

Parallel Computation of Dynamic Terrain

Thomas M. Kendall, Terry A. Purnell, and Virginia A. Kaste
U. S. Army Research Laboratory, Aberdeen Proving Ground, MD

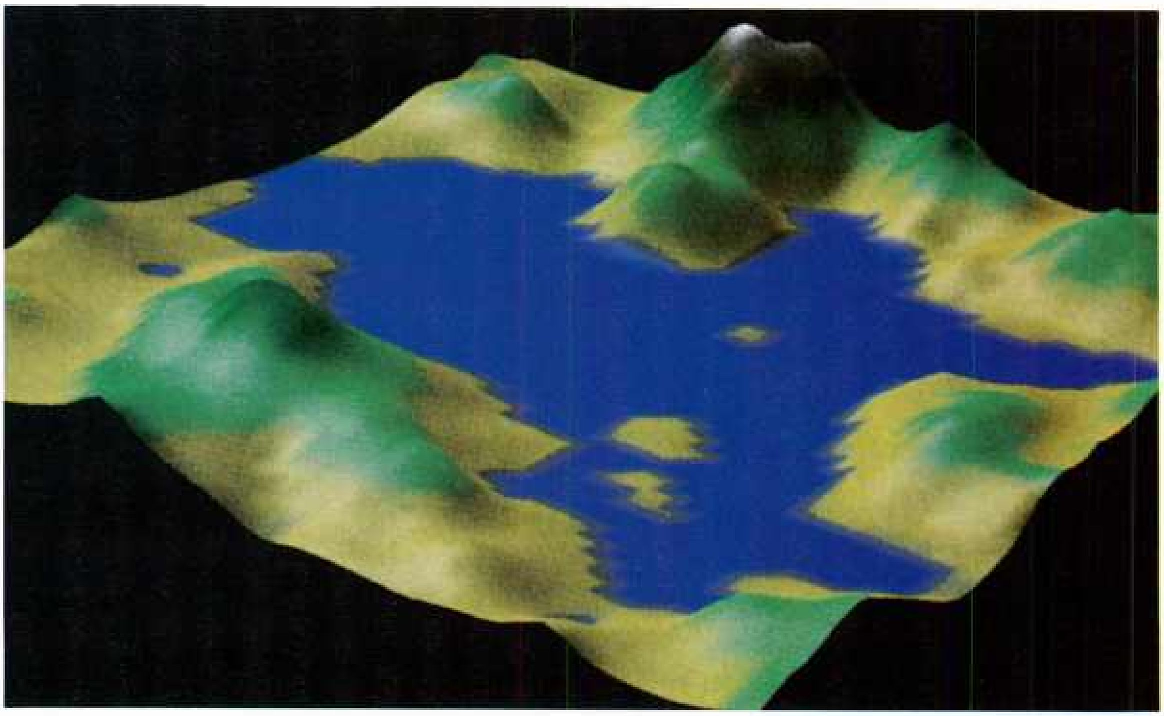
Computer Resource: TMC CM-5 [AHPCRC, Minneapolis, MN]; Intel Paragon XP/S [ASC, Wright-Patterson AFB, OH]; Cray C-90 [CEWES, Vicksburg, MS]; and Kendall Square Research KSR-1 [ARL, Aberdeen Proving Ground, MD]

Research Objective: To evaluate the performance of the Army Research Laboratory's (ARL) variable resolution terrain (VRT) model on existing massively parallel processing (MPP) computers. This will allow the computer that is best suited to the application to be used in the final implementation.

Methodology: The ARL-VRT model is used to create computer-generated terrain for use in combat simulations and synthetic environments. To provide accurate results, these applications require high-resolution dynamic terrain. The ARL-VRT model is based on the concept that terrain is made up of many hills, each with an associated set of parameters. The elevation at any point can be computed by summing over the elevation of each individual hill at that point. The methodology for implementing the model on the CM-5 and the Paragon is to assign a region of terrain to each processing element. Once the parameters are stored in the processing element's memory, no other communication is required until the computation is complete. The KSR-1 uses a shared-memory programming model; thus, no explicit message passing is required. On the C-90, only a single CPU is used.

Results: Of the four systems considered, the CM-5 was the best overall performer. The main loop executes approximately two times faster than the Paragon and seven times faster than the KSR-1, when 32 processing elements are used on each machine. The 32-node partition of the CM-5 is approximately three times faster than a single processor of the C-90.

Significance: The ARL-VRT model can be used to generate high-resolution terrain for combat simulations and synthetic environments that can be used for improved training and materiel evaluation.



Variable resolution terrain

Environmental Quality Modeling is one of the fastest growing areas of HPC within DoD. EQM involves the efficient solution of the equations of mass, momentum, energy, and constituent transport that supports environmental restoration and stewardship on DoD-managed lands. DoD has over 10,000 contaminated sites requiring restoration, and significant stewardship actions are required to manage the natural and cultural resources on DoD installations. EQM couples most (often, all) of the computational intensity associated with computational fluid dynamics with reactive, multi-phase, multi-component transport. Multiple state variables and highly nonlinear constitutive relationships are common to EQM computations.

The EQM success stories that follow were chosen from a broad range of state-of-the-art applications to illustrate the computational challenges associated with EQM and to highlight the use of EQM in real-world DoD engineering solutions. These applications, while conducted primarily by major Service laboratories, are the products of collaborative research between DoD, DoE, EPA, and academic research partners.

Environmental Quality Modeling and Simulation

Mr. Jeffrey P. Holland
Army Corps of Engineers, Waterways Experiment Station
CTA Leader for EQM

Hydrodynamic and Salinity Investigations for Strategic Waterway Modifications

R.C. Berger
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

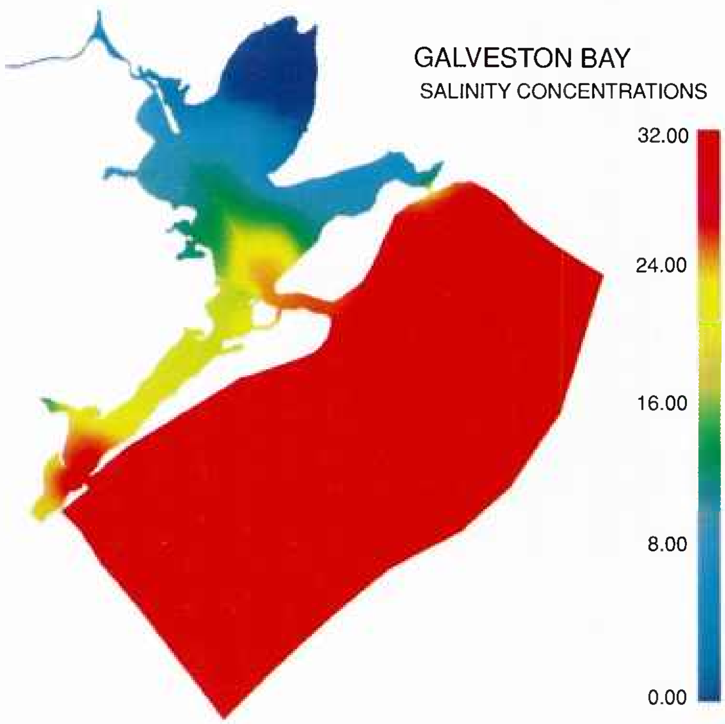
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: To investigate the potential environmental quality and circulation impacts associated with modifications to a strategic national port—the Houston-Galveston, Texas Navigation Channels Project.

Methodology: Three-dimensional calculations for hydrodynamics and salinity were computed over the entire Galveston bay system. Approximately 14,000 computational nodes were used to solve this system of highly nonlinear equations. Sharp saline and velocity fronts were routine, especially near abrupt geometric changes such as those at the channel-estuary interface. The 3-D calculations required producing and postprocessing 30 differing 9- to 12-month-long simulation scenarios that covered different geometric alignments, tide combinations, and wind conditions. The 3-D velocity and salinity fields were computed and assessed for potential impacts on the aquatic ecosystem (local mussel beds are highly sensitive to ambient salinity levels).

Results: Significant improvement has been achieved in optimizing salinity levels as a function of the proposed waterway geometry. These calculations have proven to be a direct basis for comparison of different waterway plans, and their environmental and navigation efficiencies, by federal, state, and local agencies.

Significance: This nation has thousands of miles of harbors and waterways whose navigation is essential to move troops and material during combat. Environmentally sustainable engineering management of these waterways is essential to their continued effectiveness. The dual-use modeling technology employed in this study is a key technology used by resource agencies to determine the environmental "fitness" of waterway design. Confidence in these calculations is a key to their acceptance by regulators and other decision makers. Prior to consistent access to DoD resources, the required level of confidence in 3-D calculations was not achievable because of such a large geographic scale.



Computed salinity contours from Houston-Galveston, Texas Navigation Channels Project. The colors range from red (high salinity, Gulf of Mexico) to dark blue (fresh water)

Environmental Modeling of the Chesapeake Bay

M.S. Dortch and C.F. Cerco
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

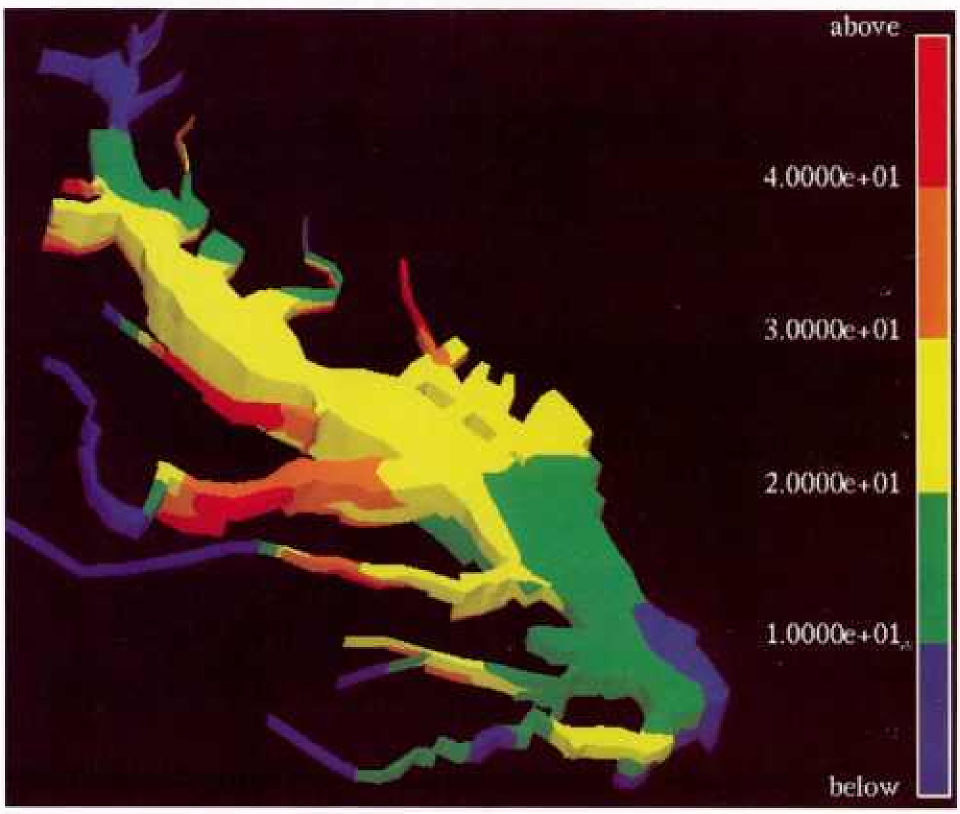
Computer Resource: Cray Y-MP [CEWES, Vicksburg, MS]

Research Objective: To predict future water quality of the Chesapeake Bay resulting from various candidate cleanup strategies.

Methodology: A three-dimensional, hydrodynamic and water quality modeling system was developed to simulate water currents and water quality constituents. The codes were written in FORTRAN77 and were optimized for vector processing. This was the first coupled, fully 3-D, time-variable hydrodynamic and water quality simulation of a large-scale estuarine/marine system.

Results: Thirty-year hind-case simulations with this model successfully predicted existing conditions in the bay. The modeling system is being used by EPA and bay states to evaluate the effectiveness of various cleanup strategies to restore health to the bay. This successful state-of-the-art model development and application has resulted in similar applications to six other large estuarine/marine systems, including the New York Bight. The modeling system could be used to evaluate the effect on receiving waters of cleanup activities of adjacent defense installations, such as the numerous military bases in the Chesapeake Bay watershed.

Significance: This new capability provides realistic evaluation of potential cleanup strategies for vast waterbodies. Its results can have significant implications for regulatory activities. This modeling system can determine not only the most cost-effective cleanup strategy but also the length of time it would take for the waterbody to respond to the cleanup. Cleanup cost for the Chesapeake Bay is estimated at $10 billion.



Computed spring algal bloom in Chesapeake Bay

Evaluation of Remediation Strategies for Military Installations

J.P. Holland and D.R. Richards
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

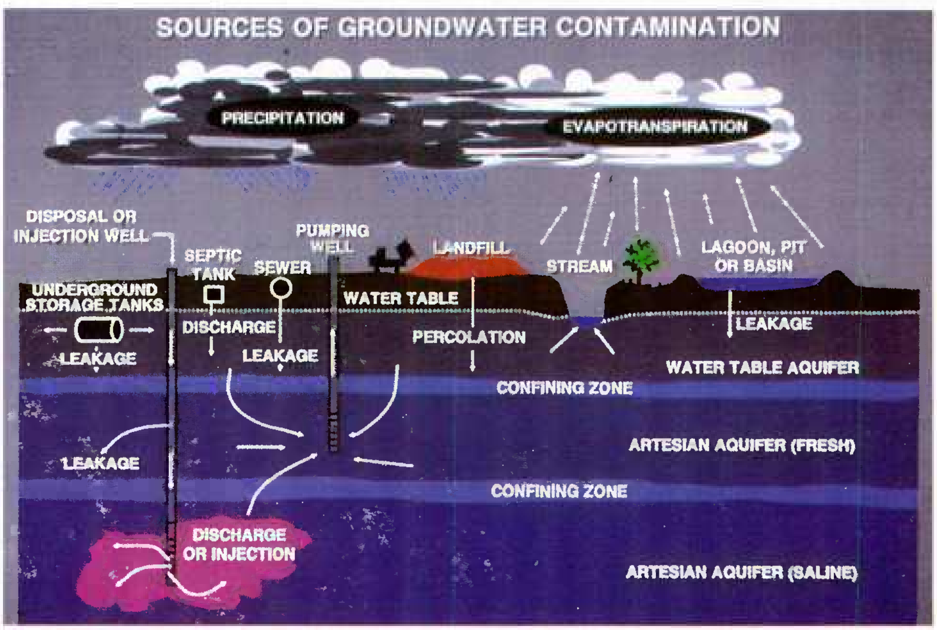
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS]

Research Objective: To develop efficient, accurate, subsurface flow and transport modeling tools in support of the large-scale cleanup of contaminated groundwater resources at military installations.

Methodology: Three-dimensional, time-varying calculations for coupled saturated-unsaturated zone subsurface flows and contaminant fate/transport for highly heterogeneous porous media were made for both specific cleanup sites and research aquifers. The calculations required solution domains comprising tens of thousands to hundreds of thousands of nodes and millions of nonlinear equations. The calculations were conducted to investigate new process descriptions and algorithms and to support actual cleanup technology design and optimization at specific sites. Calculations for many of these large sites (up to square kilometers), coupled with the large number of equations required to solve the calculations, would have been impractical or impossible without DoD HPC resources.

Results: Significant improvement has been achieved in designing remedial alternatives for specific military sites. For example, potential savings of several million dollars were achieved at a given installation through regulatory acceptance of calculations showing equivalent cleanup capabilities for a significantly simpler system design than previously required by the regulators.

Significance: DoD has over 10,000 installation sites that may require some form of cleanup caused by past contamination of groundwater resources. Contamination at these sites exists in complex hydrogeochemical environments that are highly heterogeneous physically and biochemically. The expected cleanup costs at these sites are estimated at $45 billion and growing. The ability to confidently numerically evaluate the efficacy of remedial designs and to optimize those designs over decadal time frames prior to actual implementation is an essential component of cost-effective remediation. This technology also has a direct dual use in civilian superfund cleanups.



Contaminants exist in a complex, highly heterogeneous environment subject to all of the forcings shown

Impacts of Subsurface Heterogeneity on Installation Cleanup

J. F. Peters, S. E. Howington, and J. P. Holland
U.S. Army Engineers Waterways Experiment Station, Vicksburg, MS

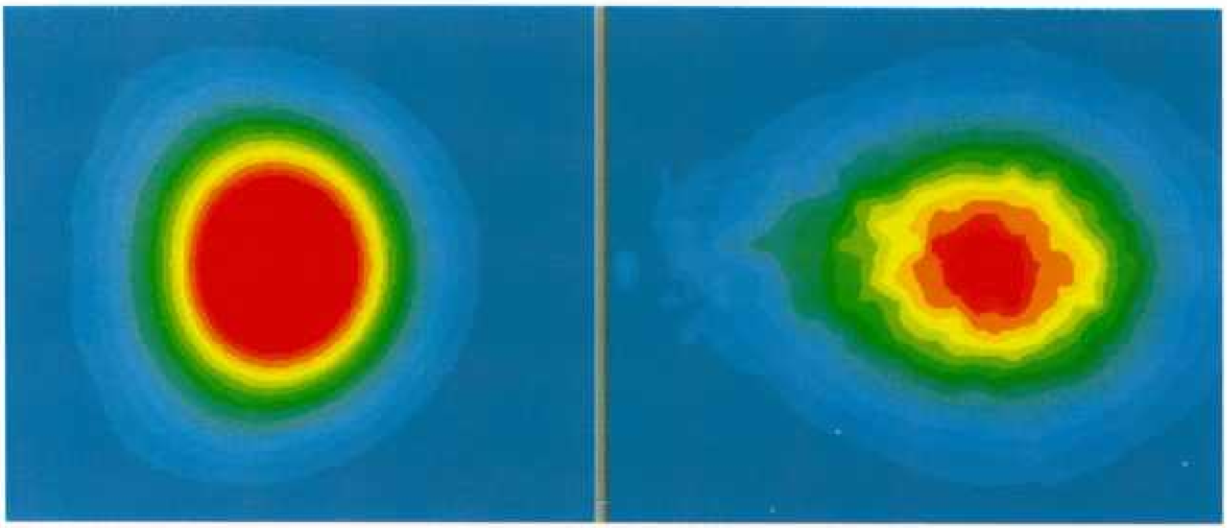
Computer Resource: Cray C-90 and Y-MP [CEWES, Vicksburg, MS] and TMC CM-5 [AHPCRC, Minneapolis, MN]

Research Objective: To create a predictive capability for transport of contaminants in heterogeneous media to support remediation of contaminated groundwater at military installations.

Methodology: Equations describing flow and transport in porous material were derived and tested to eliminate scale dependencies displayed by current models. Numerical approximations that could be applied to practical field problems were constructed for these equations. The new methods were tested by comparing them to laboratory and field data. Numerical experiments of pore-scale phenomena were used to address otherwise unobservable physical processes.

Results: Equations whose parameters are scale independent have been derived for flow and conservative transport. It was found that these equations could be approximated as advective transport through a discrete network. The network characteristics can be generated stochastically to simulate field-scale flow and dispersion. The model correctly predicts the observed growth rates of contaminant plumes that are interpreted by existing theories to be scale dependency. A key feature of this method is that a distribution of velocities and concentrations is associated with each position, rather than a single value.

Significance: The DoD has cleanup responsibility for over 10,000 sites with possible contaminated groundwater resources. The estimated cost is $45 billion. These contaminated sites are physically, chemically, and biologically heterogeneous, rendering traditional methods ineffective. These new theories and corresponding models will improve capability to predict performance of remediation schemes, an essential element of reliable remediation design. Application of these theories is not possible without HPC resources. As more physical, chemical, and biological processes are considered in applying innovative remediation schemes to actual sites, DoD HPC resources will be severely taxed.



Comparison of tracer plumes for a homogeneous dispersive medium (left), and a medium with fine-scale heterogeneity (right)

Virtually all DoD systems employ electronics, and in most cases, the very latest or leading-edge technologies. Given the importance of reliable, state-of-the-art electronics, the development, design, and analysis of electronic systems is paramount.

The Computational Electronics and Nanoelectronics group develops scalable software that lowers the costs and enables improved performance of DoD electronics through a variety of CAD/CAE and predictive modeling and simulation techniques. These tools enable the exploration of device and circuit structures without fabrication, the simulation and optimization of device and circuit concepts, and the study of the interaction between electronic components and system operation. The following contributions provide an indication of the types of improvements possible.

Computational Electronics and Nanoelectronics

Mr. David L. Rhodes
Army Research Laboratory
CTA Leader for CEN

Vortex Lattices in Unconventional Superconductors

Daryl W. Hess

Naval Research Laboratory, Washington, DC

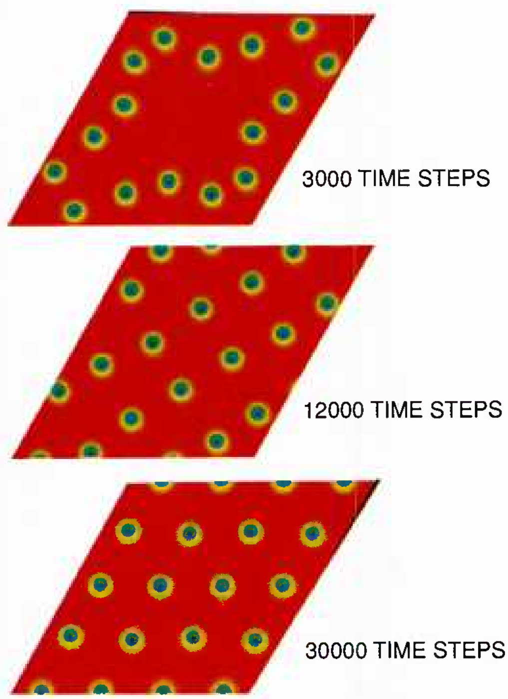
Computer Resource: TMC CM-5 [NRL, Washington, DC]

Research Objective: Conventional superconductors are described by an order parameter (OP) with two degrees of freedom; the OP for an unconventional superconductor (US) can have more degrees of freedom. This work is aimed at calculating the field-temperature phase diagram of a promising model for the superconducting state of the heavy fermion superconductor UPt_3. Experiments in the mixed state show three distinct superconducting states coexisting with weak antiferromagnetic order.

Methodology: Using a massively parallel algorithm, the Ginzburg-Landau (GL) equations are solved for a US with a complex two-dimensional vector OP (four degrees of freedom). The calculation includes a symmetry-allowed (weak) coupling of superconducting and coexistent antiferromagnetic order. The set of (seven) coupled nonlinear second order partial differential equations are solved self-consistently on a mesh for the spatial variation of the OP, magnetic field and supercurrent. The problem is particularly well suited to a computer with a parallel architecture. Because field variables at a site are directly coupled only to those on near sites, interprocessor communications are particularly efficient. A relaxation algorithm updates the OP and vector potential on the entire mesh for a time step until convergence. The GL equations are solved for fixed primitive-cell geometries; the Gibbs free energy is a minimum at the physical lattice geometry.

Results: Fixed-field vortex lattice solutions have been obtained as a function of temperature for several sets of parameters entering into the GL equations. The figure shows the formation of a vortex lattice similar to those in a conventional superconductor. As the temperature is decreased, a phase transition occurs (not shown) in which the structure of the core of each vortex abruptly changes.

Significance: The conclusive identification of a US would open a new frontier for the study and application of superconductivity. The field-temperature phase diagram of UPt_3 is unlike that of any conventional superconductor and strongly suggests that UPt_3 is a US, however, the symmetry of the order parameter is not known. The phase transition obtained in these calculations supports the physical picture of a 2-D unconventional order parameter that couples to weak antiferromagnetic order. A direct observation of the abrupt and dramatic change in vortex core structure (e.g., by scanning tunneling microscopy) would provide strong support for this picture.



Time evolution of the GL equations toward the steady state solution is summarized by the "snapshots." Starting from a homogeneous superconductor in an applied magnetic field with no flux penetration, flux tubes (vortices) rapidly penetrate the body of the superconductor and eventually form a triangular lattice. For the vortices shown here, superconductivity is strongly suppressed in the core region (blue), whereas between the vortices it is nearly that of a bulk homogeneous superconductor (red regions).

AUTHOR INDEX

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